1974

Subsurface void contrast by scanning electron microscopy: theory and applications

Joseph Kirk Gasper
Iowa State University

Follow this and additional works at: https://lib.dr.iastate.edu/rtd

Part of the Nuclear Engineering Commons

Recommended Citation
https://lib.dr.iastate.edu/rtd/6337

This Dissertation is brought to you for free and open access by the Iowa State University Capstones, Theses and Dissertations at Iowa State University Digital Repository. It has been accepted for inclusion in Retrospective Theses and Dissertations by an authorized administrator of Iowa State University Digital Repository. For more information, please contact digirep@iastate.edu.
INFORMATION TO USERS

This material was produced from a microfilm copy of the original document. While the most advanced technological means to photograph and reproduce this document have been used, the quality is heavily dependent upon the quality of the original submitted.

The following explanation of techniques is provided to help you understand markings or patterns which may appear on this reproduction.

1. The sign or "target" for pages apparently lacking from the document photographed is "Missing Page(s)". If it was possible to obtain the missing page(s) or section, they are spliced into the film along with adjacent pages. This may have necessitated cutting thru an image and duplicating adjacent pages to insure you complete continuity.

2. When an image on the film is obliterated with a large round black mark, it is an indication that the photographer suspected that the copy may have moved during exposure and thus cause a blurred image. You will find a good image of the page in the adjacent frame.

3. When a map, drawing or chart, etc., was part of the material being photographed the photographer followed a definite method in "sectioning" the material. It is customary to begin photoing at the upper left hand corner of a large sheet and to continue photoing from left to right in equal sections with a small overlap. If necessary, sectioning is continued again — beginning below the first row and continuing on until complete.

4. The majority of users indicate that the textual content is of greatest value, however, a somewhat higher quality reproduction could be made from "photographs" if essential to the understanding of the dissertation. Silver prints of "photographs" may be ordered at additional charge by writing the Order Department, giving the catalog number, title, author and specific pages you wish reproduced.

5. PLEASE NOTE: Some pages may have indistinct print. Filmed as received.

Xerox University Microfilms
300 North Zeeb Road
Ann Arbor, Michigan 48106
GASPER, Joseph Kirk, 1948-
SUBSURFACE VOID CONTRAST BY SCANNING ELECTRON MICROSCOPY: THEORY AND APPLICATIONS.

Iowa State University, Ph.D., 1974
Engineering, nuclear

Xerox University Microfilms, Ann Arbor, Michigan 48106

THIS DISSERTATION HAS BEEN MICROFILMED EXACTLY AS RECEIVED.
Subsurface void contrast by scanning electron microscopy:
Theory and applications

by

Joseph Kirk Gasper

A Dissertation Submitted to the
Graduate Faculty in Partial Fulfillment of
The Requirements for the Degree of
DOCTOR OF PHILOSOPHY

Department: Chemical Engineering and Nuclear Engineering
Major: Nuclear Engineering

Approved:

Signature was redacted for privacy.

In Charge of Major Work
Signature was redacted for privacy.

For the Major Department
Signature was redacted for privacy.

For the Graduate College

Iowa State University
Ames, Iowa

1974
### TABLE OF CONTENTS

| NOTATION | iv |
| INTRODUCTION | 1 |
| LITERATURE REVIEW | 10 |
| THEORETICAL DEVELOPMENT | 20 |
| The Monte Carlo Method | 20 |
| Simulation of the Interactions Between Electrons and Materials Using the Monte Carlo Method | 22 |
| Geometry Used in the Monte Carlo Calculations | 26 |
| Single Scattering Theory | 30 |
| Multiple Scattering Theory | 40 |
| Secondary Electron Production Theory | 50 |
| COMPUTATIONAL TECHNIQUES | 55 |
| Model Used in the Simulation of Electron Interactions in a Specimen Containing a Void | 55 |
| Monte Carlo Method Computer Algorithm | 58 |
| Subsurface Void Analysis Computer Algorithm | 67 |
| RESULTS AND DISCUSSION | 77 |
| Cases Used to Test the Validity of the Monte Carlo Method Computer Programs | 77 |
| Calculation of Subsurface Void Contrast | 100 |
| Examination of a Specimen Containing Voids Using the SEM | 121 |
| Monte Carlo Method Applied to Multiple Element Systems | 135 |
iii

CONCLUSIONS 139

SUGGESTIONS FOR FURTHER RESEARCH 151

LITERATURE CITED 156

ACKNOWLEDGMENTS 164

APPENDIX A: PROGRAMS USED IN THE ANALYSIS OF SUBSURFACE VOID CONTRAST 165

Monte Carlo Method Programs 165

Single scattering Monte Carlo program 169
Multiple scattering data program 188
Combined single and multiple scattering theory Monte Carlo program 199

Secondary Electron Production Programs 229

Subsurface Void Analysis Program 241

APPENDIX B: SINGLE SCATTERING THEORY AND COMPUTER ALGORITHM FOR COMPOUNDS AND ALLOYS 268
### NOTATION

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>( A )</td>
<td>atomic weight</td>
</tr>
<tr>
<td>( A_j )</td>
<td>atomic weight of element ( j )</td>
</tr>
<tr>
<td>( a_0 )</td>
<td>first Bohr radius</td>
</tr>
<tr>
<td>( C_i )</td>
<td>expansion term used to calculate ( \kappa_i )</td>
</tr>
<tr>
<td>( C_j )</td>
<td>weight fraction of element ( j )</td>
</tr>
<tr>
<td>( c )</td>
<td>velocity of light</td>
</tr>
<tr>
<td>( dS )</td>
<td>differential electron path length</td>
</tr>
<tr>
<td>( \frac{dE}{dS} )</td>
<td>energy loss per unit path length</td>
</tr>
<tr>
<td>( - \frac{dn}{n(S)} dS )</td>
<td>the probability that an electron not scattered in traversing a distance ( S ) will be scattered between ( S ) and ( S + dS )</td>
</tr>
<tr>
<td>( \frac{d\sigma(\beta)}{d\Omega} )</td>
<td>Rutherford scattering cross section</td>
</tr>
<tr>
<td>( \frac{d\sigma_j(\beta)}{d\Omega} )</td>
<td>Rutherford scattering cross section for element ( j )</td>
</tr>
<tr>
<td>( d\Omega )</td>
<td>solid angle</td>
</tr>
<tr>
<td>( E )</td>
<td>electron energy</td>
</tr>
<tr>
<td>( E_0 )</td>
<td>electron rest mass energy equivalent</td>
</tr>
<tr>
<td>( E_{\text{max}} )</td>
<td>maximum energy loss in one inelastic collision</td>
</tr>
<tr>
<td>( E_n )</td>
<td>electron energy at the point of the ( n_{\text{th}} ) elastic collision</td>
</tr>
<tr>
<td>( e )</td>
<td>electronic charge</td>
</tr>
<tr>
<td>( F_S(\beta) )</td>
<td>integral probability function of scattering in single scattering theory</td>
</tr>
<tr>
<td>( F_s(S) )</td>
<td>single scattering integral probability scattering function</td>
</tr>
</tbody>
</table>
$F_m(\beta)$ integral probability function of scattering in multiple scattering theory

$f(\beta)$ differential probability function of scattering in multiple scattering theory

$f_k(\beta)$ intensity of electrons which have suffered exactly $k$ collisions while scattering through the angle $\beta$

$h(S^*)$ the probability for a secondary electron to move towards and escape from the specimen surface

$\hbar$ reduced Planck's constant

$I$ mean ionization potential

$I, \bar{j}, \bar{k}$ coordinate system with respect to the incident beam

$K$ constant used to determine $\Delta S_n$

$I, \bar{m}, \bar{n}$ coordinate system with respect to the previous scattering direction

$m$ mass of the electron

$N$ number of atoms per unit volume

$N_j$ atoms per unit volume of element $j$

$N_0$ Avogadro's number

$N\sigma(E)$ macroscopic cross section

$n_0$ number of incident electrons

$n_t$ number of electrons emerging from a specimen of thickness $t$

$n(E)$ number of electrons with energy less than or equal to $E$

$n(S)$ number of electrons traveling a distance $S$

$n(S) \frac{n(S)}{n_0}$ the probability that an incident electron has not scattered in traversing a distance $S$ in the material

$n_s(S)\, dS$ number of secondary electrons produced by one incident electron along a path length between $S$ and $S+dS$
$P_i$ Legendre polynomial of the first kind of order $i$

$P_e$ number of elastic scattering collisions in one multiple scattering step

$p(\beta)$ multiple scattering probability of scattering through an angle $\beta$

$p_s(S)$ single scattering collision probability as a function of path length

$Q$ amount of energy loss

$Q_i$ Legendre polynomial of the second kind of order $i$

$r$ electron position

$R$ random number

$S$ electron path length

$S^*$ path length of a secondary electron to the surface

$t$ sample thickness

$v$ velocity of the electron

$W_k$ the probability of an electron experiencing exactly $k$ collisions before leaving a specimen

$Z$ atomic number

$Z_j$ atomic number of element $j$

$z$ depth of the electron below the surface of the specimen

$\alpha$ azimuthal scattering deflection

$\alpha'$ secondary electron attenuation coefficient

$\beta$ polar scattering deflection

$\beta_j$ screening angle used in Rutherford cross section

$\beta_{s,j}$ screening angle of element $j$

$\Delta$ number of secondary electrons
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Delta S_n$</td>
<td>step length for the $n_{th}$ step in the Monte Carlo simulation</td>
</tr>
<tr>
<td>$\delta$</td>
<td>secondary electron coefficient = number of secondary electrons / number of incident electrons</td>
</tr>
<tr>
<td>$\delta_n$</td>
<td>secondary electron coefficient of the backscattered electrons</td>
</tr>
<tr>
<td>$\delta_p$</td>
<td>secondary electron coefficient of the incident electrons</td>
</tr>
<tr>
<td>$\varepsilon_e$</td>
<td>secondary electron excitation energy</td>
</tr>
<tr>
<td>$\eta$</td>
<td>backscattering electron coefficient</td>
</tr>
<tr>
<td>$\theta$</td>
<td>polar scattering angle</td>
</tr>
<tr>
<td>$\theta_n$</td>
<td>scattering angle $\theta$ after the $n_{th}$ collision</td>
</tr>
<tr>
<td>$\kappa_i$</td>
<td>a measure of the probability of electron scattering in multiple scattering theory</td>
</tr>
<tr>
<td>$\lambda$</td>
<td>incident electron mean free path</td>
</tr>
<tr>
<td>$\lambda_j$</td>
<td>incident electron mean free path in element $j$</td>
</tr>
<tr>
<td>$\lambda_s$</td>
<td>secondary electron mean free path</td>
</tr>
<tr>
<td>$\nu$</td>
<td>chance of a single collision between the electron and the atom</td>
</tr>
<tr>
<td>$\rho$</td>
<td>material density</td>
</tr>
<tr>
<td>$\sigma(E)$</td>
<td>energy dependent microscopic cross section for electron collisions</td>
</tr>
<tr>
<td>$\Sigma$</td>
<td>summation</td>
</tr>
<tr>
<td>$\phi$</td>
<td>azimuthal scattering angle</td>
</tr>
<tr>
<td>$\phi$</td>
<td>scattering angle $\phi$ after the $n_{th}$ collision</td>
</tr>
<tr>
<td>$\psi(E,Q)$</td>
<td>probability per unit path length per energy interval that an electron will lose an amount of energy $Q$</td>
</tr>
<tr>
<td>$\vec{\Omega}$</td>
<td>direction of electron travel</td>
</tr>
</tbody>
</table>
INTRODUCTION

The analysis of cavities in reactor materials is a major topic for understanding the properties of materials in the reactor environment. This includes the analysis of fission gas bubbles in ceramic and metallic fuels during normal and transient operation of thermal and fast reactors. These bubbles play a role in the life of the fuel and the safe operation of these reactors. Analysis of cavity formation in metals for use as cladding and other structural materials is of equal importance. This includes void formation in potential fast reactor cladding materials and blistering of potential controlled thermonuclear fusion reactor first wall materials. Prior to the introduction of the Scanning Electron Microscope (SEM) all analyses were performed using either an optical microscope or a transmission electron microscope. The introduction of the SEM gave the researcher an instrument with a wide range of magnifications and great depth of field. The bulk of cavity analysis using the SEM has been for intermediate magnification (2000X to 10,000X) studies of gas bubbles. The SEM has not been used extensively at higher magnifications because it has an operational resolution limit on the order of 150 Å while the transmission electron microscope, with an operational resolution limit on the order of 30 Å, is much more useful in studying the initial phases of
cavity formation. However, with the introduction of the field emission electron source an operation resolution limit on the order of 50 Å can be obtained in the SEM and examination of cavities at high magnification becomes practical using the SEM.

The SEM offers the researcher several important features not available in the transmission electron microscope. The SEM can handle large bulk specimens which can eliminate the need to thin radioactive specimens. Also the SEM has a very large depth of field. This makes it possible to study large pieces of irregularly shaped material at high magnification.

In order to interpret the micrographs of materials containing cavities it is necessary to understand the signal formation process that takes place in the SEM. The SEM works on the principle that when an electron beam strikes a specimen a variety of signals are produced, including backscattered electrons, secondary electrons, X-rays, and Auger electrons, which are detected and visually displayed in the form of a picture. The first two of these signals are primarily used in the topographical analysis of the specimen while the latter two are primarily used in the chemical analysis of the specimen. In this work the signal formed by the backscattered and secondary electrons is studied. The photomicrograph is formed in the SEM by synchronously rastering the electron beam over
the surface of the specimen and the electron beam of a cathode ray tube (CRT) over the phosphorescent screen. The amplitude of the CRT beam is determined by the strength of the signal received by the detector. The picture formed by this method corresponds to an optical picture of the specimen. The contrast in a SEM micrograph is proportional to the variation in strength of the signal received by the detector.

There are two primary contrast mechanisms for secondary and backscattered electron Scanning Electron Micrographs. The first of these is due to the slope of the specimen with respect to the incident beam. Everhart et al. (1) have shown that an alteration in surface inclination of only one or two degrees would generally be sufficient to cause an appreciable change in brightness of the final image using secondary electrons. A second contrast mechanism is due to the variation in chemical composition of the specimen. This is due to the unique backscattering and secondary electron coefficient of each element and any variation in the elemental make up of different sections of the specimen results in a variation in the yield of backscattering and secondary electrons from sections of the specimen. In a specimen containing cavities both contrast mechanisms may be visible in the micrographs. If the cavity is open on the surface of the specimen the sides of the cavity vary in slope with respect to the incident electron beam. An additional surface contrast mechanism
may be visible in SEM micrographs. This is the absorption of secondary and backscattered electrons by the sides of the cavity so that fewer electrons reach the detector from the cavity than from the rest of the specimen. The contrast due to changes in the elemental composition or atomic number occurs when a cavity lies below the surface of the specimen. The contrast results from the difference between the atomic number of the cavity and the atomic number of the surrounding material. The fact that subsurface atomic number contrast is visible in SEM photomicrographs has been demonstrated by Kimoto and Hashimoto (2). This contrast results from the interaction between backscattered electrons and the subsurface cavity. Since the cavities are of a low atomic number, as compared to that of the surrounding material, the backscattering coefficient of the cavity is low and the combined backscattering coefficient of the subsurface cavity and the material surrounding it is less than the backscattering coefficient of the solid material. The fact that subsurface features can be seen in Scanning Electron Micrographs has been demonstrated by Greer (3). Wells (4) has shown that large subsurface cavities are visible in secondary electron SEM micrographs. The purpose of this work is to better understand the role of subsurface cavities in the formation of the backscattered and secondary electron signals in the SEM.
theoretical analysis using the Monte Carlo method is carried out to help understand the interactions between the incident electrons and the subsurface cavities. An experimental analysis is done to confirm the theoretical results and to study the image formed by subsurface cavities.

The Monte Carlo method was chosen to analyze subsurface void contrast because of the great variety of cases that can be analyzed using this method and because of the previous successful application of this method to the theory of SEM image formation. This method can provide information about contrast for both secondary and backscattered electron signals. The method can handle a wide variety of void geometries, specimen chemical compositions, electron beam energies, and specimen geometries. The computer programs using this method compute contrast variation that can be qualitatively compared to SEM photomicrographs of subsurface voids.

The Monte Carlo method is used to simulate the interaction between the incident beam of electrons and the specimen by simulating the trajectories of individual electrons in the specimen and combining a large number of these electron histories to obtain a picture of the interactions between the specimen and the beam. The Monte Carlo method simulates the inelastic and elastic collisions that the incident electrons suffer during their passage through the material.
The inelastic scattering between incident electrons and atomic electrons is simulated using the Bethe continuous energy loss theory. This theory determines the energy of the incident electrons as they pass through the material. The electron position and direction of travel are determined by the scattering of the incident electrons by the nucleus and the path length the electron travels between elastic collisions. Two theories can be used to simulate these interactions. Single scattering theory simulates collisions between the electron and the nucleus. The path length is related to the electron's mean free path length. Multiple scattering theory simulates a series of elastic collisions in a single step of the model and the step length is determined by the number of elastic collisions that occur in that distance. The single scattering theory provides the fine details of the electron interactions but executes slowly on the computer. Multiple scattering theory provides a more gross picture of the electron interactions but executes more rapidly on the computer than the single scattering theory. Both theories use the screened Rutherford scattering cross section to determine the scattering direction in a collision between the electron and the atom.

Previously both theories have been used in Monte Carlo method simulations of the interaction between the electron beam and the specimen. Multiple scattering theory Monte
Carlo calculations have been used to analyze characteristic X-ray production in a sample, backscattered electron energy distribution, depth of electron penetration, broadening of the electron beam in the specimen, and secondary electron production. Single scattering theory has been used to analyze backscattering of electrons by thin films, backscattered electron spatial distribution, incident electron energy dissipation, and characteristic X-ray production. Both theories have been shown to be adequate to simulate backscattering electron properties with the single scattering theory being more precise. However, multiple scattering theory calculations have not been successful in accurately simulating secondary electron production.

One of the purposes of this study is to extend the usefulness of the Monte Carlo method for the simulation of the interaction between electrons and the specimen by using a combined single and multiple scattering theory Monte Carlo method algorithm. This algorithm uses the best features of both theories. Single scattering theory is used in the region of the specimen near the surface where secondary electrons are produced and where incident electrons cross boundaries separating physically different regions. This provides the algorithm with the most accurate simulation in regions where an accurate simulation is required. Multiple scattering theory is used where the incident electrons are below the region of
secondary electron production and in homogeneous regions. This provides the algorithm with a rapid simulation of the interactions in regions of the specimen where it is not necessary to know the details of the electron history. The necessary equations for single and multiple scattering theory are derived and are used in an algorithm which simulates the interactions between the electrons and the specimen using the IBM 360-65 computer.

This algorithm is applied to the problem of subsurface void contrast. The analysis is performed for a copper specimen with an incident electron energy of 20 keV. Before the subsurface void analysis can be performed the programs are tested using published data and expressions are chosen for the variables used in the single and multiple scattering equations. In order to choose these values a single scattering theory program is used to simulate electron scattering by thin films. By comparing this calculated data with experimental data, the program is tested and the expression for the term that accounts for the screening of the nucleus by atomic electrons is chosen. By comparing this data with values of the multiple scattering theory cross section for various angles of scattering the multiple scattering cross section program is tested and the number of elastic collisions simulated by a multiple scattering step is determined.

The combined single and multiple scattering theory pro-
gram is used to produce backscattered electron histories that are stored on magnetic tape. A semiquantitative theory of secondary electron production is used to calculate secondary electron yield of these histories. A program is developed which calculates the backscattering and secondary electron coefficients for a copper specimen containing various size parallelepiped voids using the recorded histories. These coefficients are used to calculate the theoretical contrast ratios for subsurface voids. Based on an analysis of this data for copper it is possible to predict the contrast effects of subsurface voids for other specimens and electron energies.

These calculated results are compared with SEM micrographs of subsurface voids in a doped tungsten filament to check the ability of the algorithm to simulate this type of interaction. The micrographs are also used to characterize the subsurface voids. Because the algorithms are designed for specimens composed of single element regions and because many specimens of interest to the nuclear engineer are compounds or alloys a modified single scattering theory algorithm is derived. This algorithm is checked against experimental results for a copper gold alloy.
LITERATURE REVIEW

The Scanning Electron Microscope (SEM) is a good tool to study the microstructural properties of reactor materials. This is because bulk specimens may be examined at intermediate and high magnification with little or no sample preparation. Because of this the SEM has been used and is being used to examine ceramic and metallic nuclear materials. The examination is usually carried out on fracture surfaces or cross sections of the material. Examination of materials containing cavities has been done for irradiated ceramic nuclear fuel, stainless steel, and potential first wall materials for the controlled thermonuclear reactor (CTR).

Reynolds and Bannister (5) studied the fracture surfaces of irradiated UO₂ fuel using the SEM. They observed bubbles ranging from 0.2 μm to 2.0 μm on the exposed grain surfaces and they observed bubble linkage along the grain edges. They demonstrated that the SEM is a satisfactory tool for examining the nature of grain boundary porosity in irradiated UO₂.

Dapht, Pati, and Boyle (6) used the SEM in conjunction with replica and thin foil techniques to study the kinetics of fission gas re-solution in UO₂ irradiated in a fast neutron flux. The re-solution of fission product gasses at elevated temperatures was studied by Turnbull and Cornell (7) using the SEM and transmission electron microscope to observe the
fission gas microbubbles and to measure the efficiency of the re-solution process. Turnbull (8) studied the effect of grain size on the swelling and gas release properties of UO$_2$ during irradiation. He observed polished sections and fracture surfaces of the irradiated fuel in the SEM to analyze bubble formation and migration to grain boundaries. He also observed bubble linkage on the grain boundaries. Turnbull calculated the percentage of swelling in the material by measuring the bubble size and distribution on the surface of the grains. Burton and Reynolds (9) used the SEM to examine the fracture surfaces of sintered uranium dioxide to determine the residual porosity of the material after sintering. They observed that the majority of the micro-pores were situated along grain boundaries.

Much of the examination of fission gas morphology in ceramic fuels uses replica techniques. Micheis and Dragel (10) prepared a report on the preparation and examination of these replicas. However, the resolution of this replica technique is limited to about 500 Å. A SEM with 100 Å resolution capability is presently being installed at Argonne National Laboratory to examine fast reactor fuel elements (11). They expect to use the SEM in conjunction with the transmission electron microscope replicas to examine failed fast reactor fuel elements.

Besides the examination of ceramic materials, the SEM
has been used to study the performance of metals in the reactor environment. This includes the study of cladding and structural materials for the liquid metal fast breeder reactor and first wall materials for a controlled thermonuclear reactor. Hunter, Fish, and Holmes (12) used the SEM in a study of channel fracture of type 304 stainless steel irradiated in the Experimental Breeder Reactor II (EBR II). They observed plastic dimpling fracture resulting from the formation of microvoids at inclusions by homogeneous shear and the growth of these microvoids by continuous homogeneous shear of the metal between the microvoids. Sandusky, Armizo, and Wagner (13) used the SEM to study the pitting of types 316 and 321 stainless steels due to the long term exposure to liquid sodium. They observed some linkage between these pits and what were thought to be subsurface cavities between the grains.

Several researchers have studied the implantation and re-emission of gasses from metal surfaces. Bauer and Thomas (14) used the SEM to study the surfaces and cross sections of helium implanted palladium. They used the SEM to observe the large bubbles on the surface of the palladium and the development of submicron gas bubbles at the implanted layer in the specimen. Bauer and Thomas (15) used the SEM to examine the helium bubbles in niobium, vanadium, and molybdenum. The helium was injected at different temperatures and to different
concentrations in the material. They examined the movement and coalescence of the microbubbles as a function of temperature. Kaminsky and Das (16) used the SEM to study the effect of material temperature on the degree of blistering for different wall materials (e.g., Nb, V, and type 304 stainless steel).

The SEM has been used to examine materials containing cavities at intermediate (2,000X) and high magnifications (20,000X). In all these examinations the cavities have been assumed to be on the surface of the specimens. However, this study will attempt to show that the interpretation of the high magnification micrographs requires the consideration that some of the cavities are below the specimen surface. The introduction of the field emission source SEM should increase the use of the SEM at high magnifications making a correct interpretation of high magnification micrographs of specimens containing cavities more important.

The interpretation of these micrographs requires an understanding of the signal formation process in the SEM. The signal in the SEM results from the interaction between the electron beam and the specimen. An understanding of the interaction and the resulting signals can be obtained by experimental techniques, using specially prepared specimens, or by theoretical techniques. Both methods have been used
but the theoretical techniques are better developed and provide a fundamental understanding of the interaction between the electron beam and the specimen. These theoretical techniques have been applied to Scanning Electron Microscopy and this has lead to an improved understanding of the signal formation process in the SEM. This understanding allows better interpretation of Scanning Electron Micrographs.

Extensive literature exists on the theory of the interaction between charged particles and materials. Bomback (17) has reviewed the literature on the interactions between electrons and solids and summarized the basic interactions that must be understood to interpret Scanning Electron Micrographs. He includes a bibliography of theoretical and experimental work on the interactions of electrons and solids. Zerby and Keller (18) reviewed electron transport theory, calculations, and experiments with emphasis on estimating the radiation that would penetrate a space craft. Their review is for electrons in an energy range below 10 MeV. Wittry (19) briefly reviews the basic electron beam interactions in solids and applies the results obtained by theory and by experiment to the various signals that can be obtained in the SEM. He includes a discussion of resolution and contrast of the secondary and backscattered electron signals in the SEM. These three articles give a basic discussion of the theory of interactions between electrons and solids, but they do not
include a detailed discussion of the calculational techniques that can be used to better understand these interactions in the SEM. The most widely used calculational method is the Monte Carlo method. This method provides the most detailed information about the interactions between electrons and solids, and gives results that compare favorably with experimental results. It is necessary to use either transport theory or Monte Carlo methods to accurately analyze the interactions between the electron beam and the specimen. Cosslett and Thomas (20) found that the simple theories of electron interactions with solids do not favorably compare with experimental results and only the more complex methods could be used to obtain theoretical results that favorably compare with the experimental results.

Monte Carlo calculational techniques have been used to simulate the electron interactions with the specimen in the SEM. Monte Carlo calculations trace the paths of individual electrons to obtain a simulation of the electron interactions with the specimen. Berger (21) reviews the various theories and calculational techniques that can be used in Monte Carlo method simulations of the penetration and diffusion of charged particles. He includes discussions of various Monte Carlo schemes, computational aspects, and solutions of typical problems. Investigators have used several different Monte Carlo schemes to obtain satisfactory simulations of the
interaction between the electron beam and the specimen. These schemes can be broken down into two broad classes: single scattering theory schemes and multiple scattering theory schemes. The single scattering theory scheme simulates each elastic collision with a step in the Monte Carlo calculation while the multiple scattering theory scheme simulates a series of elastic collisions with a single step of the Monte Carlo calculation.

An experimentally based multiple scattering theory Monte Carlo simulation was used by Green (22) to study the spatial distribution of characteristic X-ray production in a copper target with an incident electron energy of 29 keV. In this model the polar scattering angle is determined from tables of scattering data for thin copper films of various thicknesses for an incident electron energy of 29 keV. Bishop (23) used Green's technique to study the backscattered electron energy distribution, average depth of electron penetration, and characteristic X-ray production for a copper specimen with 29 keV incident electrons.

Reiner, Gilde, and Sommer (24) use a multiple scattering technique which assumes a constant number of elastic scattering collisions per step taken in the Monte Carlo calculation to study the broadening of an electron beam in a specimen for incident electron energies of 17 to 1200 keV. Shinoda, Murata, and Shimizu (25) use this constant number of scattering
collisions approximation in their Monte Carlo calculations based on Lewis' multiple scattering theory (26). They use this technique to study the backscattering electron and characteristic X-ray production for several elements with several incident electron energies. Shimizu, Honji, and Murata (27) use this technique to study energy dissipation of electrons in aluminum and copper targets. Shimizu, Ikuta, Nishigori, and Murata (28) use this technique to calculate characteristic X-ray production in alloy targets. Shimizu and Murata (29) apply this technique to understanding the fundamentals of the SEM and the Electron Probe Microanalyzer. They obtain backscattering and secondary electron coefficients that agree with experimental data and they obtain lateral distributions of backscattered and secondary electrons. Shimizu, Ikuta, and Murata (30) use a modification of their existing technique to improve their multiple scattering algorithm to obtain better agreement with experimental data. They also analyzed the relationship between the depth at which an electron backscattered and the energy of the backscattered electron. Nishigori, Shimizu, and Murata (31) use a multiple scattering theory Monte Carlo simulation to study quantitative X-ray microanalysis of alloy systems. Bishop (32) uses the constant number of scattering events approximation in Monte Carlo calculations based on the Goudsmit and Saunderson multiple scattering theory to study electron penetration in
several single element specimens.

Curgenven and Duncumb (33) developed a multiple scattering scheme that assumes a constant energy loss for each step in the Monte Carlo calculation. They give some preliminary results using this scheme. Bolon and Lifshin (34) use this Monte Carlo technique to study X-ray analysis of thin films and fine structure.

Monte Carlo calculations based on single scattering theory have been less extensively used to simulate the interaction between the electron beam and the specimen. McDonald, Lamki, and Delaney (35) use this theory to study the backscattering of electron beams by thin films. Murata, Matsukawa, and Shimizu (36) use single scattering theory Monte Carlo calculations to study backscattered electrons, energy dissipation, characteristic X-ray production, and secondary electron emission for aluminum, copper, and gold targets. Shimizu and Everhart (37) use this model to study the energy dissipation of electrons in an organic specimen. Murata (38) uses this theory to study the spatial distribution of backscattered and secondary electrons in the SEM.

One purpose of this study is to develop a computer algorithm that uses the best features of both the single and multiple scattering theory. One would like to retain the accuracy of simulating each elastic collision by using the single scattering theory model while retaining the
calculational speed of the multiple scattering theory Monte Carlo calculations. This computer algorithm is discussed in the Computational Techniques section. This algorithm is applied to the problem of subsurface void contrast in the SEM which is an important phenomenon to understand in order to interpret Scanning Electron Micrographs of cavities in reactor materials.
THEORETICAL DEVELOPMENT

The Monte Carlo Method

The Monte Carlo method originated during the early 1940's as a result of suggestions advanced by J. von Neumann and S. Ulam at Los Alamos. However, virtually nothing appeared in the literature until about 1949. In that year the first symposium on Monte Carlo methods was held at Los Angeles under the sponsorship of the RAND Corporation and the National Bureau of Standards (NBS) in cooperation with Oak Ridge National Laboratory. The proceedings of this conference were published by NBS (39) in 1951. Since its beginnings the Monte Carlo method has been used extensively to simulate the transport and diffusion of neutrons and charged particles through material. There are many references which describe the general details of the Monte Carlo method. These include Clark and Hansen (40), Lattès (41), and Hammersley and Handscomb (42). Rather than further develop the general method, this work will concentrate on the Monte Carlo method for the simulation of electron interactions with the specimen.

Since the electron interactions with a solid are described by electron cross sections, which are in essence probabilities of interactions, the Monte Carlo technique can be applied to investigate the electron interactions with the specimen. The path length of the electron and the angles of scattering
are determined by electron cross sections of the material. The cross section data must be obtained by experiment or theory for the material in order to utilize the Monte Carlo method.

The Monte Carlo method is based on the assumption that the interaction between the electron beam and the specimen can be analyzed by simulating the passage of each individual electron through the specimen and summing these to obtain a picture of the electron interactions with the specimen. Each electron is given an initial position, energy, and direction of travel. The individual electron is followed through a series of collisions until it crosses the specimen surface and backscatters, until its energy falls below a certain minimum, or until it reaches a depth below which the probability of the electron backscattering is very small. The latter two restrictions are used to prevent the electron from being followed too long and to keep the execution time of the computer simulation reasonable.

The above process is repeated over and over for a large number of electrons, each of which produces a history of the electron interactions. By combining the histories, it is possible to simulate the actual physical behavior of the electron beam interacting with the specimen. This probabilistic treatment does not have the generality of an analytical solution but it corresponds closely to the process of electron
interactions in matter which is probabilistic in nature.

Simulation of the Interactions Between Electrons and Materials Using the Monte Carlo Method

The Monte Carlo method must simulate all possible interactions between the incident electrons and the atoms in the specimen. The incident electrons undergo inelastic collisions with the atomic electrons. The incident electron undergoes a great number of these inelastic collisions and they may be thought of as a continuum of collisions. The incident electron can be visualized as continuously slowing down as it penetrates the specimen. As the incident electrons collide with the atomic electrons some of the atomic electrons may receive sufficient energy to escape from the atom and the specimen. These escaped electrons are secondary electrons.

The incident electrons undergo elastic and inelastic collisions with the nucleus of the specimen atoms. This leads to scattering of the incident electrons which is described by the Rutherford cross section. Because the nucleus of the specimen atom is effectively screened from the incident electrons by the atomic electrons the classic Rutherford cross section must be modified in order to account for this screening.
Another mechanism for interaction between an electron and an atom is the Bremsstrahlung interaction. In these interactions the incident electron loses energy through the production of X-rays. However, it has been shown that this interaction becomes negligible for electron energies of less than a few MeV. This interaction will not be considered in these calculations since the SEM normally operates at electron energies of less than 50 keV.

The Monte Carlo method is used to simulate the movement of the electron through the specimen by simulating the various interactions between the incident electrons and the specimen atoms. The major assumptions of the Monte Carlo method for the simulation of charged particle interactions are (1) the scattering centers are distributed at random, although not necessarily with a uniform density, throughout the specimen, and (2) the charged particle, in the course of traversing the specimen, interacts with one scattering center at a time. The trajectory of the particle is thus an idealized zig-zag path, consisting of free flights interrupted by sudden collisions in which the direction of the particle is changed.

The trajectory of a particle is described by an array

\[ E_0, E_1, E_2, \ldots, E_n, \ldots \]

\[ \theta_0, \theta_1, \theta_2, \ldots, \theta_n, \ldots \]
where $E_n$ is the energy, $\vec{\eta}_n$ is the direction, and $r_n$ is the position of the electron after the $n$th collision, and where the index zero refers to the initial state of the electron. Such a trajectory can be generated by Monte Carlo calculations using random sampling. The probability distribution for transition from one state to the next, i.e. from one column of the array to the next, is determined by single scattering probabilities.

Because of the strength and the long range of the Coulomb interaction the number of collisions in a typical charged particle history is enormous. Several thousand collisions may be required in order to adequately describe a case history. However, when it is necessary to describe the fine details of a case history, this type of analysis must be used.

To reduce the required amount of computation we abandon the complete description of charged particle histories and limit ourselves to "snapshots" taken at various times during the particle's history. A series of "snapshots" provides a "moving picture" of the history which can be used to describe the electron interactions with the material. In order to select the times at which the snapshots are to be taken it is convenient, although not absolutely necessary, to use as a
clock the path length traveled by the electron. Thus the condensed case histories are introduced

\[ 0, S_1, S_2, \ldots, S_n, \ldots \]
\[ E_0, E_1, E_2, \ldots, E_n, \ldots \]
\[ \Omega_0, \Omega_1, \Omega_2, \ldots, \Omega_n, \ldots \]
\[ r_0, r_1, r_2, \ldots, r_n, \ldots \]

where \( E_n \) is the energy, \( \Omega_n \) is the direction, and \( r_n \) is the position of the electron when it has traveled a path length \( S_n \) from its starting point. A condensed history is sampled by letting the electron carry out a random walk in which each step, from state \( n \) to \( n+1 \), takes into account the combined effect of many collisions. The transition probabilities for each step are determined by the appropriate multiple scattering theories. There would be no question as to how this random walk should be carried out if a complete theory were available, but then the Monte Carlo calculations themselves would become unnecessary. The important point is that even incomplete and partial theories, when suitably combined, can yield enough information so that condensed case histories can be sampled with fair accuracy.

Two types of Monte Carlo calculations have been introduced: one using detailed case histories and the other using condensed case histories. The detailed case history technique
uses single scattering theory while the condensed case history technique uses multiple scattering theory. Before describing single and multiple scattering theory and energy loss theory in detail it is necessary to derive the geometric relationships that are used to keep track of the position and direction of travel of the electron during its history.

Geometry Used in the Monte Carlo Calculations

The geometry used in the Monte Carlo calculations is shown in Figure 1. Let \( \vec{\Omega}_n(\theta_n, \phi_n) \) and \( \vec{\Omega}_{n+1}(\theta_{n+1}, \phi_{n+1}) \) denote the directions of the electron at the beginning and end of a step, and \( \beta \) and \( \alpha \) denote the polar and azimuthal scattering deflections in that step. The direction at the beginning of the step is given by

\[
\vec{\Omega}_n = \sin \theta_n \cos \phi_n \vec{i} + \sin \theta_n \sin \phi_n \vec{j} + \cos \theta_n \vec{k} \tag{3}
\]

where \( \vec{i}, \vec{j}, \) and \( \vec{k} \) are unit vectors in the Cartesian coordinate system and \( \theta \) and \( \phi \) are spherical coordinates in a system with the \( Z \) axis as the polar axis. The new direction, \( \vec{\Omega}_{n+1} \), is defined in terms of a coordinate system \( \vec{i}, \vec{m}, \) and \( \vec{n} \) and angles \( \alpha \) and \( \beta \) are defined with respect to a spherical coordinate system whose polar axis coincides with the direction of motion at the beginning of the step

\[
\vec{n} \equiv \vec{\Omega}_n.
\]
Figure 1. Geometry used in the Monte Carlo calculations
\( \beta \) represents the angle between \( \vec{n} \) and \( \vec{n}_{n+1} \). The angle \( \alpha \) is the angle between the \( \vec{I} \) axis and the projection of the new direction of travel in the \( \vec{l} \cdot \vec{m} \) plane. The new direction can be written

\[
\vec{n}_{n+1} = \sin \beta \cos \alpha \vec{I} + \sin \beta \sin \alpha \vec{m} + \cos \beta \vec{n}
\]  

(4)

where

\[
\vec{n} = \sin \theta_n \cos \phi_n \vec{I} + \sin \theta_n \sin \phi_n \vec{J} + \cos \theta_n \vec{K}
\]  

(5)

The vector \( \vec{m} \) can be related to the \( \vec{I} \), \( \vec{J} \), and \( \vec{K} \) coordinate system by

\[
\vec{m} = \sin \phi_n \vec{I} - \cos \phi_n \vec{J}
\]  

(6)

and

\[
\vec{l} = \vec{m} \times \vec{n} = (-\cos \phi_n \cos \theta_n) \vec{I} - (\sin \phi_n \cos \theta_n) \vec{J}
\]

\[+ \sin \theta_n \vec{K}
\]  

(7)

By substituting Equations 5, 6, and 7 into Equation 4 and by rearranging, one obtains

\[
\vec{n}_{n+1} = [-\sin \beta \cos \alpha (\cos \phi_n \cos \theta_n) + \sin \beta \sin \alpha (\sin \phi_n) \\
+ \cos \beta (\sin \theta_n \sin \phi_n)] \vec{I} \\
+ [-\sin \beta \cos \alpha (\sin \phi_n \cos \theta_n) - \sin \beta \sin \alpha (\cos \phi_n) \\
+ \cos \beta (\sin \theta_n \sin \phi_n)] \vec{J} \\
+ [\sin \beta \cos \alpha (\sin \theta_n) + \cos \beta (\cos \theta_n)] \vec{K}.
\]  

(8)
Thus $\vec{\Omega}_{n+1}$ is defined in terms of both the spherical coordinates of the direction of motion at the beginning of the step and the spherical coordinates of the coordinate system with the polar axis coinciding to the direction of motion at the beginning of the step and can be utilized in a term by term comparison with

$$
\vec{\Omega}_{n+1} = \sin \theta_{n+1} \cos \phi_{n+1} \vec{I} + \sin \theta_{n+1} \sin \phi_{n+1} \vec{J} + \cos \theta_{n+1} \vec{K}.
$$

(9)

This leads to the well known kinematic relations between the change of direction and the scattering deflections.

$$
\cos \theta_{n+1} = \cos \theta_n \cos \beta + \sin \theta_n \sin \beta \cos \alpha
$$

(10)

$$
\sin(\phi_{n+1} - \phi_n) = \sin \beta \sin \alpha / \sin \theta_{n+1}
$$

(11)

$$
\cos(\phi_{n+1} - \phi_n) = (\cos \beta - \cos \theta_{n+1} \cos \theta_n) / (\sin \theta_n \sin \theta_{n+1})
$$

(12)

These equations are utilized in the Monte Carlo calculations for both the single and multiple scattering theory models.
Single Scattering Theory

In order to use single scattering theory, expressions are needed for the path length between collisions, the scattering angles $\alpha$ and $\beta$, and the loss of incident electron energy. The first consideration is to determine the probability of an elastic scattering event occurring as a function of distance traveled by the electron. The probability, $p(S)\,dS$, where $p(S)$ is defined as the collision probability, that the electron will experience a discrete event, such as an elastic scattering event, and an attendant change in direction in traversing a distance between $S$ and $S+dS$ is given by

$$p(S)\,dS = [-dn/n(S)]\left[n(S)/n_0\right]dS$$

(13)

where

$$-dn/n(S)\,dS \equiv \text{the probability that an electron not scattered in traversing a distance } S \text{ will be scattered between } S \text{ and } S+dS, \text{ and}$$

$$n(S)/n_0 \equiv \text{the probability that an incident electron has not been scattered in traversing a distance } S \text{ in the material.}$$

These definitions are made assuming that multiple scattering resulting in a previously scattered electron re-entering the beam is negligible.

The collision probability is related to the energy dependent cross section. If an individual target atom presents
a cross-sectional area, $\sigma(E)$, to the incoming electrons, then assuming that the electron field does not shield the nucleus, the total collision area presented by a target of thickness $dS$ with $N$ atoms per unit volume is given by $\sigma(E)NdS$. The fraction of beam electrons which interact in traversing thickness $dS$ is then given by

$$-\frac{dn}{n(S)}dS = \sigma(E)NdS$$

(14)

This equation can be dealt with analytically if a unique relationship between $E$ and $S$ can be assumed or if the slab is sufficiently thin so that the variation of $\sigma(E)$ with $S$, and hence $E$, can be neglected. The latter condition requires that

$$\left| \frac{\sigma(S) - \sigma(0)}{\sigma(S)} \right|$$

$$= \left| \frac{d\sigma(E)/dE}{dE/dS}/\sigma(E) \right|_{E=E_0}$$

(15)

where $S$ is small.

This results in a simple solution to Equation 14:

$$n(S) = n_0 \exp[-\sigma(E_0)NS].$$

(16)

Equations 13, 14, and 16 can be combined to give

$$p(S) = \sigma(E) N \exp[-\sigma(E_0)NS]dS.$$ 

(17)

The integral probability function is defined for single scattering as
\[ F_s(S) = \int_0^S p(S') dS' \quad (18) \]

and represents the probability that an electron will be scattered in a distance \( S \). The quantity \( F_s(S) \) ranges from zero to one for all \( S \) and thus generation of a random number between zero and one defines a unique distance the electron travels between collisions. For the collision probability described by Equation 18 \( F_s(S) \) is given by

\[ F_s(S) = 1 - \exp[-\sigma(E_0)NS]. \quad (19) \]

The mean free path between collisions is defined as

\[ \lambda = \int_0^\infty S'p(S')dS', \quad (20) \]

where \( S' \) is a dummy of integration, which when combined with Equation 17 yields

\[ \lambda = \frac{1}{N\sigma(E)}. \quad (21) \]

Therefore, the probability of scattering as a function of path length is related to a physically known quantity, the mean free path.

The next step is to consider the angular probabilities of the scattering event. It is desired to know the probability of the electron scattering in the direction \( \vec{n} \) after an interaction with an atom. The case of a charged particle being scattered by a nuclear field was first considered by
Rutherford for the case of alpha particles and this same analysis can be carried out for electrons. This analysis assumes that the electron is scattered only by the electrostatic field associated with the nucleus and neglects the effect of atomic electrons. The Rutherford cross section can be derived using either classical or wave mechanics. Kaplan (43) gives the derivation using classical mechanics and Mott and Massey (44) give the derivation using wave mechanics. Rather than repeating the derivation here the resulting expression for the cross section is given here:

$$
\frac{d\sigma(\beta)}{d\Omega} = \left[ \frac{Z^2 e^4}{4E^2} \right] (1 - \cos \beta)^{-2} .
$$

(22)

As can be seen the cross section can be described as a function of $\beta$ only and it is independent of $\alpha$. The range of values of $\beta$ is from zero to $\pi$ and $\alpha$ ranges from zero to $2\pi$. Here the factor for inelastic collisions has been neglected because the probability that electrons are influenced by inelastic collisions with large angle scattering is small compared to that of elastic collisions if the atomic number is not very low. In the case of light elements, this effect is not negligible, and $Z^2$ in Equation 22 should be replaced by $Z(Z+1)$ according to the theory derived by Kulchitsky and Latychev (45). The solid angle $d\Omega$ is defined as
\[ d\Omega = \sin \beta d\theta d\alpha \]

in the spherical coordinate system and the integral cross section, \( \sigma(E) \), can be defined as

\[ \sigma(E) = 2\pi \int_{0}^{\pi} [d\sigma(\beta)/d\Omega] \sin \beta d\beta. \quad (23) \]

Next the integral probability of an electron scattering into a solid angle \( d\Omega \) is defined as

\[ F_{S}(\beta) = \left[ 1/\sigma(E) \right] \int_{0}^{2\pi} \int_{0}^{\pi} [d\sigma(\beta')/d\Omega] \sin \beta' d\beta' d\alpha \quad (24) \]

where \( d\sigma(\beta)/d\Omega \) is defined by Equation 22 and \( \sigma(E) \) by Equation 23.

The derivations given in Kaplan and Mott and Massey for Equation 22 assume that the nucleus appears as a point charge with its associated Coulomb field to the approaching electron. This assumption neglects the fact that the nucleus is surrounded by a cloud of electrons that effectively screens the approaching electron from the nucleus. In order to account for this Wentzel (46) has suggested that the Rutherford cross section can be corrected by inserting a screening angle term into Equation 22. The screened Rutherford cross section is

\[ d\sigma(\beta)/d\Omega = \left( \frac{Z^2 e^4}{4\pi \varepsilon^2} \right) \left[ 1 - \cos \beta + 2\beta_{s} \right]^{-2}, \quad (25) \]

where \( \beta_{s} \) is the screening angle. Several authors have
derived expressions for $\beta_s$. Wentzel (46) derived an expression:

$$\beta_{sw}^{1/3} = \left( \frac{Mz}{mv \alpha_0} \right)^2. \quad (26a)$$

Mott and Massey (44) derived an expression using the first Born approximation and a Hartree field:

$$\beta_{sm}^{1/3} = \left[ 0.373Z (e^2/\hbar\nu) \right]^2. \quad (27a)$$

Molière (47) derived an expression which he claims is valid using the second Born approximation and a Thomas-Fermi field:

$$\beta_{sm}^{1/3} \alpha_0 \left( \frac{Mz}{0.885 mva_0} \right)^2 \left[ 1.13+3.76\left( \frac{Z/137(\nu/c)}{\nu/c} \right)^2 \right] \quad (28a)$$

Nigam et al. (48), however, claim that Molière has made some errors in his derivation and claim that Molière's expression is only good for cases where the first Born approximation is valid. Nigam et al. derive a new expression for the screening angle using the second Born approximation and a Thomas-Fermi field:

$$\beta_{sn} = 0.25 \left[ 1.12 \left( \frac{M}{m} \right) \left( \frac{Z}{\nu} \right) \right] \left( \frac{Z}{\nu} \right)^{1/3} \alpha_0 \left( \frac{Mz}{0.885 mva_0} \right)^2. \quad (29a)$$

By making the substitutions

$$a_0 = \frac{M^2}{me^2}$$
$$\frac{e^2}{\hbar} = \frac{e^2e_0E^{-1/2}}{\sqrt{2} Mc}$$
and
\[ E_0 = 0.511 \times 10^6 \text{ ev} \]

into Equations 26a, 27a and 29a the following expressions for \( \beta_s \) can be obtained:
\[
\beta_{sw} = 3.402 Z^{2/3} E^{-1} \quad (26b)
\]
\[
\beta_{sm} = 1.891 Z^{2/3} E^{-1} , \text{ and} \quad (27b)
\]
\[
\beta_n = 5.449 Z^{2/3} E^{-1} . \quad (29b)
\]

Neglecting the second term of Molière's expression and making the same substitutions a similar expression can be obtained:
\[
\beta_{sm} = 4.908 Z^{2/3} E^{-1} . \quad (28b)
\]

Several more cross section expressions have been derived to take into account more theoretical effects [see for example Spencer (49)]. However, these expressions are much more difficult to utilize in the calculations and the calculational errors associated with the present form of the cross section are felt to dominate. Therefore, additional refinements should lead to only a minor increase in accuracy with a large increase in computation time. The choice of which
form of $\beta_s$ to use in Equation 25 will be discussed in a later section.

Equation 24 determines the polar angle of scattering due to elastic collisions but the direction of electron travel, $\vec{\Omega}_n$, is a function of both $\alpha$ and $\beta$. It is assumed that the scattering through the azimuthal angle, $\alpha$, is uniformly distributed between zero and $2\pi$ and that it is independent of energy.

Expressions have been derived to determine the electron path length between elastic collisions and the direction of electron travel after an elastic collision. According to Equation 1 an expression is needed to determine the electron energy at the point of each elastic collision in order to utilize a single scattering theory Monte Carlo method computer algorithm. The incident electron loses energy as a result of inelastic collisions with atomic electrons. The collisions are assumed to have a negligible effect on the direction of travel. As the electron passes through a medium it collides with atomic electrons, and on each of these collisions there is a finite probability that another electron will be set in motion. Hence, the incident electron loses its energy in a series of finite steps, a certain portion of which produce secondary electrons. After a collision, since it is impossible to say which electron was incident on the other, the most energetic is assumed to be the
incident electron. Thus the energy loss of the incident electron is limited to not more than one half of its energy at each collision.

For electron energies of interest in the SEM it can be assumed that the electron undergoes a great many small energy loss collisions as it passes through a solid. These small energy loss collisions can be treated using continuous energy loss theory. The average energy loss per unit path length is given by

$$\frac{dE}{dS} = \int_{E}^{E_{\text{max}}} Q\psi(E,Q)dQ$$

where $\psi(E,Q)$ is the probability per unit path length per energy interval that an electron will lose an amount of energy, $Q$, by a collision in a given material. To integrate Equation 30 it is necessary to assume that the first Born approximation holds and that $E_{\text{max}}$ is not too great (e.g., $E_{\text{max}} \ll E$). Even with these assumptions the integration of Equation 30 is quite complex and involves the use of momentum variables and the optical model of two body collisions. Bethe (50) carried out this integration as part of a general energy loss theory and the resulting equation is

$$-\frac{dE}{dS} = (2\pi e^4 N Z / E) \ln(2E/I)$$

where $I$ is the mean ionization potential. This expression is
not quite correct because insufficient consideration has been given to the ultimate indistinguishability of the two electrons emerging from the ionizing collision. If the maximum energy loss is $E/2$ then the energy loss in the logarithmic term in Equation 31 is $E/2$ and not $E$. With the Mott cross section for identical particles of spin 1/2, Bethe and Ashkin (51) give a modified energy loss equation

$$-\frac{dE}{dS} = \frac{2\pi e^{-4NZ/E}}{4\ln(\sqrt{e/2} E/I)} \tag{32}$$

where $e$ in the logarithmic expression is the natural base of the logarithms. The value of $I$ used in the calculations is obtained from Duncumb and Reed (52). The difference between Equation 31 and Equation 32 does not usually amount to more than ten percent.

This completes the derivation of the equations necessary to formulate a single scattering theory Monte Carlo method algorithm. The algorithm will be given in the Computational Techniques section. The next subject to be considered in this section is the theory necessary to formulate a multiple scattering theory Monte Carlo method algorithm.
Multiple Scattering Theory

Multiple scattering theory Monte Carlo calculations simulate a series of elastic scattering events in a single step of the Monte Carlo calculations. To carry out this simulation requires the development of a new angular scattering equation and a new step length determining equation. The Bethe continuous energy loss equation is used to determine the electron energy at the beginning and end of each step.

The multiple scattering theory of Goudsmit and Saunder-son (53, 54) is used in this model. This theory is based on the fact that the angular distribution of electrons which suffer exactly k collisions can be determined exactly with respect to their initial direction provided they remain in the same homogeneous medium and provided they do not lose a significant fraction of their initial energy. The latter assumption is valid for a thin section of material provided no large energy loss events occur. The difficulty arises in the statistical nature of the collision events because electrons leaving the thin section may have experienced a small or large number of collisions and the angular distribution of electrons leaving the section represents a combination of the various angular distributions related to specific numbers of collisions. The derivation of the theory is given by Goudsmit and Saunderson (53, 54) and Mott and Massey (44) and an
outline of it is given here.

To determine the angular distribution of electrons after exactly $k$ collisions it is necessary to define

$$f_k(\Omega)d\Omega = \text{intensity of electrons which have suffered exactly } k \text{ collisions within the solid angle } d\Omega \text{ about direction } \Omega,$$

and

$$p(\Omega_1+\Omega)d\Omega = \text{probability that an electron with initial direction } \Omega_1 \text{ will be scattered into a solid angle } d\Omega \text{ about the direction } \Omega.$$

In accordance with these definitions $f_{k+1}(\Omega)$ is related to $f_k(\Omega)$ by

$$f_{k+1}(\Omega) = \int_{d\Omega_1} f_k(\Omega)p(\Omega_1+\Omega)d\Omega_1d\Omega. \quad (33)$$

Since

$$\cos \beta = \Omega_1 \cdot \Omega$$

$p(\Omega_1+\Omega)$ is a function of $\beta$ only and $p(\beta)$ can be expanded in terms of Legendre polynomials so that

$$p(\beta) = (2\pi)^{-1} \sum_{i=0}^{\infty} (2i+1/2)g_iP_i(\cos \beta). \quad (34)$$

g_i is obtained by multiplying Equation 34 by $d\Omega$ and integrating

$$g_i = 2\pi \int_{0}^{\pi} p(\beta)P_i(\cos \beta) \sin \beta d\beta. \quad (35)$$

The angular distribution, $f_1(\Omega)d\Omega$, is given by
\[ f_1(\Omega) d\Omega = f_1(\beta) \sin \beta d\beta d\alpha \]

\[ = [(2\pi)^{-1} \sum_{i=1}^{\infty} \frac{(2i+1)}{2} g_i P_i(\cos \beta_1)] \sin \beta d\beta d\alpha \]

(36)

which is a function of \( \beta \) only. To find \( f_2(\beta) d\Omega \) Equations 33, 34, and 36 are used to obtain

\[ f_2(\beta) \sin \beta d\beta d\alpha = \]

\[ (2\pi)^{-2} \int_{0}^{2\pi} \int_{0}^{2\pi} \sum_{i=0}^{\infty} \{ \sum_{j=0}^{i} \frac{(2i+1)}{2} g_j P_j(\cos \beta_1) \} \sin \beta_1 \sin \beta d\beta_1 d\alpha d\beta d\alpha \]

(37)

where

\[ \cos \beta_2 = \cos \beta \cos \beta_1 + \sin \beta \sin \beta_1 \cos(\alpha_1-\alpha). \]

Using the formula

\[ P_i(\cos \beta_2) = P_i(\cos \beta) P_i(\cos \beta_1) \]

\[ + \sum_{j} \frac{(i-j)}{j(i+j)} P_i^j(\cos \beta) P_i^j(\cos \beta_1) \cos j(\alpha-\alpha_1) \]

in Equation 37 and carrying out the integrations over \( \alpha \) one obtains
\[
\int f_2(\beta) \sin \beta d\beta \, d\alpha
\]
\[
= (2\pi)^{-1} \int_0^\pi \left\{ \sum_{i=0}^\infty [(2i+1)/2] g_i P_i(\cos \beta) \right\} \sin \beta_1 d\beta_1 \sin \beta d\beta \, d\alpha
\]

and carrying out the integration over the angle \( \beta_1 \) yields

\[
f_2(\beta) = (2\pi)^{-1} \sum_{i=0}^\infty [(2i+1)/2] g_i^2 P_i(\cos \beta)
\]

where \( g_i \) is defined by Equation (35). This can be repeated to show in general that

\[
f_k(\beta) = (2\pi)^{-1} \sum_{i=0}^\infty [(2i+1)/2] (g_i)^k P_i(\cos \beta).
\]

Let \( W_k \) denote the probability of an electron experiencing exactly \( k \) collisions before leaving a thin specimen. Then

\[
f(\beta) = \sum_{k=0}^\infty W_k f_k(\beta)
\]

where \( f(\beta) \) is the normalized intensity of electrons scattering through an angle \( \beta \) and \( f(\beta) \sin \beta d\beta \) is the normalized probability that an electron will be deflected into an angle between \( \beta \) and \( \beta + d\beta \).
The problem now is to obtain a suitable expression for $W_k$. The assumption is made that the electrons have suffered a sufficient number of collisions so that multiple scattering theory applies. In this case $W_k$ is a Poisson distribution where the probability of an electron experiencing $k$ scatters is

$$W_k = e^{-v} \frac{v^k}{k!} \quad (40)$$

where $v$ is the chance of a single collision. Using Equation 40 in Equation 39 and inserting Equation 38 for $f_k(\beta)$ results in the expression

$$f(\beta) = (4\pi)^{-1} \sum_{k=0}^{\infty} \sum_{i=0}^{\infty} (2i+1)(e^{-v} \frac{v^k}{k!} g_i) P_i(\cos \beta). \quad (41)$$

The term $v^k g_i / k!$ is recognized as the Taylor's series expansion for an exponential so that Equation 41 becomes

$$f(\beta) = (4\pi)^{-1} \sum_{i=0}^{\infty} (2i+1) \exp[-v(l-g_i)] P_i(\cos \beta). \quad (42)$$

The chance of a single collision is given by

$$v = N t \sigma(E) \quad (43)$$

where $N$ is the number of atoms per unit volume, $t$ is the thickness of the specimen, and $\sigma(E)$ is the single scattering cross section.

In order to evaluate $g_i$, given in Equation 35, $p(\beta)$ is
taken to be the total differential cross section for scattering through an angle \( \beta \) such that

\[
p(\beta) = N_t \frac{d\sigma}{d\Omega}
\]

where \( \frac{d\sigma}{d\Omega} \) is the single scattering differential cross section. Inserting this expression in Equation 35 leads to the expression

\[g_i = 2\pi N_t \int_0^\pi \left[ \frac{d\sigma}{d\Omega} \right] P_i(\cos \theta) \sin \beta d\beta \tag{44}\]

Inserting Equations 43 and 44 into the expression in the exponential term of Equation 41 one obtains

\[
\nu(1-g_i) = N_t \sigma(E) - 2\pi \int_0^\pi \left[ \frac{d\sigma}{d\Omega} \right] P_i(\cos \theta) \sin \beta d\beta \]

Using Equation 23 for \( \sigma(E) \) one obtains

\[\nu(1-g_i) = 2\pi N_t \int_0^\pi \left[ \frac{d\sigma}{d\Omega} \right] [1-P_i(\cos \theta)] \sin \beta d\beta \tag{45}\]

One can define

\[
\kappa_i = 2\pi N_t \int_0^\pi \left[ \frac{d\sigma}{d\Omega} \right] [1-P_i(\cos \theta)] \sin \beta d\beta \tag{46}\]

and

\[t = \int_0^S ds\]

Inserting these expressions and Equation 45 into Equation 42 one obtains

\[f(\beta) = (4\pi)^{-1} \sum_{i=0}^\infty [(2i+1) P_i(\cos \beta) \exp(-\kappa_i \int_0^S ds)]. \tag{47}\]
Next \( S \) is approximated by \( \Delta S \), where \( \Delta S \) is a finite step. Therefore, Equation 47 becomes

\[
f(\beta) = (4\pi)^{-1} \sum_{i=0}^{\infty} (2i+1) \exp(-\kappa_i \Delta S) P_i(\cos \beta)
\]

(48)

where \( f(\beta) \) is the differential probability of an electron scattering between angles \( \beta \) and \( \beta + \Delta \beta \). To obtain the integral probability of scattering through an angle \( \beta \) it is necessary to integrate Equation 48 over the angle \( \beta \). Defining \( F_m(\beta) \) as the integral probability of scattering one obtains

\[
F_m(\beta) = \int_{0}^{\beta} f(\beta') \sin \beta' d\beta'
\]

(49)

where \( \beta' \) is the dummy of integration. This integral can be evaluated by making use of a recursion formula for Legendre polynomials

\[
P_{i+1}(\cos \beta) - P_{i-1}(\cos \beta) = (2i+1) P_i(\cos \beta) \quad i > 0
\]

where the primed quantities represent the first derivatives of \( P_i \) with respect to \( \cos \beta \). Carrying out this integration one obtains

\[
F_m(\beta) = \frac{1}{2} \sum_{i=1}^{\infty} \exp(\kappa_i \Delta S) [\frac{P_{i+1}(\cos \beta) - P_{i-1}(\cos \beta)}{2i+1}]
\]

\[+ \frac{1}{2} (1 - \cos \beta).\]

(50)

\( F_m(\beta) \) is the integral probability function for multiple
scattering theory and has values from zero to one for the values of $\beta$ from zero to $\pi$. This is the expression that is used in the Monte Carlo calculations to determine the polar angle of scattering.

The next step is to evaluate the expression for $\kappa_i$. Using the expression for the screened Rutherford scattering cross section in Equation 26 one obtains

$$
\kappa_i = \frac{2\pi N Z^2 e^4}{4E^2} \int_0^\pi \sin \beta d\beta \{[1-\cos \beta + 2\beta_s]^{-2}[1-P_i(\cos \beta)]\}
$$

It is convenient to define

$$
C_i = \int_0^\pi \sin \beta d\beta \{[1-\cos \beta + 2\beta_s]^{-2}[1-P_i(\cos \beta)]\}
$$

Spencer (49) has derived an expression for $C_i$ using Legendre polynomials of the second kind. The new expression for $C_i$ is

$$
C_i = -\frac{\beta [Q_0(1+2\beta_s)-Q_i(1+2\beta_s)]}{\beta(2\beta_s)}
$$

where $Q_i$ is a Legendre polynomial of the second kind. Making use of the recursion relationships for Legendre polynomials one obtains

$$
C_{i+1} = (2+i^{-1})(1+\beta_s) C_i -(1+i^{-1})C_{i-1} -(2+i^{-1})(1+\beta_s)^{-1}
$$

where $C_0=0$ and
\[ C_1 = \ln(1 + \beta_s^{-1}) - (1 + \beta_s)^{-1}. \]

This completes the derivation for the integral cross section for the polar scattering angle \( \beta \). The azimuthal scattering angle, \( \alpha \), is again assumed to be evenly distributed between zero and \( 2\pi \).

Next, it is necessary to obtain an expression for the path length the electron travels between multiple scattering collisions. An empirical equation is given by Cosslett and Thomas (55) in which the number of scattering events, \( p_e \), is related to the path length \( \Delta S_n \) and the electron energy at the start of the path. The expression for \( \Delta S_n \) is

\[ \Delta S_n = \frac{(p_e A E_n)}{(30 Z^{4/3} \rho)} \quad (54) \]

where \( \Delta S_n \) is in Å, \( E_n \) is in eV, and \( \rho \) is in g/m/cm\(^3\). Therefore, if \( p_e \) is specified then the path length is directly related to the energy at the start of the path such that

\[ \Delta S_n = KE_n \]

and

\[ \Delta S_{n+1} = KE_{n+1} \]

where

\[ K = \frac{(p_e A)}{(30 Z^{4/3} \rho)}. \]

Therefore, the ratio of successive path lengths is equal to the ratio of energies immediately before the \( n \)th collision and
immediately before the n+1 collision and

\[ \Delta S_{n+1} = \Delta S_n \left( \frac{E_{n+1}}{E_n} \right) . \]  \hfill (55)

The path length between elastic collisions and energy of the electron at the point of the elastic collision is determined by the choice of the initial energy of the electron and the number of elastic scattering events to be modeled by one multiple scattering step.

The usual method employed in multiple scattering Monte Carlo calculations is to allow the electron to undergo an elastic collision after traveling a path length \( \Delta S_n \) at energy \( E_{n+1} \). However, since the step length used in the multiple scattering theory algorithm is fixed by the electron energy at the start of the step, the randomness between collisions is eliminated. Since multiple scattering may be thought of as a model of single scattering this is an undesirable feature because there is a randomness of path length between elastic collisions in single scattering theory Monte Carlo calculations. To retain this randomness the electron is allowed to travel a portion of the multiple scattering step length, determined by multiplying the step length by a random number between zero and one, before undergoing an elastic collision and then it travels the remainder of the path along the new direction after the
elastic collision. This more closely approximates the situation in single scattering theory.

This completes the derivation of the equations necessary to formulate a multiple scattering theory Monte Carlo method algorithm. The algorithm is given in the Computational Technique section and then combined with the single scattering theory to formulate the combined single and multiple scattering theory Monte Carlo method algorithm.

Secondary Electron Production Theory

Since many SEM photomicrographs are made using the secondary electron signal it is desirable to be able to calculate the secondary electron yield for both the solid specimen and a specimen containing a void. A semi-quantitative theory of secondary electron production has been derived by Salow (56) and Bruining (57). An outline of this theory is given by Dekker (58). This theory is used to calculate the secondary electron coefficient using the histories produced by the Monte Carlo calculations.

It is convenient to divide the process of secondary electron production into two parts. In the first part one considers the production of secondaries resulting from the interaction between the primary electron and the lattice atoms. The second stage is the calculation of the probability that the secondaries so produced will escape from the specimen.
Thus, in a simplified way, and without paying attention to the velocity distribution of the secondaries, one may write for the secondary yield

$$\Delta = \int n_S(S)h(S^*)dS.$$  \hspace{1cm} (56)

Here $n_S(S)dS$ represents the number of secondaries produced by one primary electron along a path length between $S$ and $S+dS$; $h(S^*)$ represents the probability for such a secondary electron to move toward and escape from the surface. The integration can be carried out over the entire path length the primary electrons travel; although, only a thin layer of the specimen near the surface contributes to the production of secondaries that actually leave the specimen. The number of secondary electrons produced is proportional to the energy loss suffered by the primary electron:

$$n(S) = (-1/\varepsilon_e)(dE/dS)$$ \hspace{1cm} (57)

where $\varepsilon_e$ represents the average excitation energy required to produce a secondary electron and $dE/dS$ is the energy loss per unit path length. The probability of a secondary electron produced along the path of the primary electron escaping from the surface is determined by the exponential absorption law,

$$h(S^*) = h(0) \exp(-\alpha'S^*)$$ \hspace{1cm} (58)
where \( h(0) \) is the probability of escape for a secondary electron at or near the surface, \( S^* \) is the path length traveled by a secondary electron to get to the surface, and \( \alpha' \) is the attenuation coefficient. If one makes the approximation that the secondary electrons travel in straight lines to the surface one can state that \( \alpha' = \frac{1}{\lambda_s} \) where \( \lambda_s \) is the mean free path of the secondary electrons. For secondary electrons there is no simple way to determine \( S^* \) so that \( S^* \) is approximated with \( z \), the perpendicular distance between the point of secondary electron production and the surface. This approximation will yield a larger number of secondaries than the use of \( S^* \) but this should not seriously affect the total calculations since the approximation is consistent in all cases. Therefore, Equation 58 becomes

\[
h(S^*) = h(0) \exp\left(-\frac{z}{\lambda_s}\right)
\]

and making the use of the geometric relation

\[
z = S \cos \theta
\]

one then obtains

\[
h(S^*) = h(0) \exp\left(-S \cos \theta/\lambda_s\right).
\] (59)

Inserting Equations 57 and 59 into Equation 56 one obtains

\[
\Delta = \int \left(\frac{1}{e_g}\right) (-dE/dS) h(0) \exp\left(-S \cos \theta/\lambda_s\right) dS.
\] (60)
The integral in Equation 60 can be broken up into a series of integrals so that each integration is carried out over the individual steps of the electron histories as calculated by the Monte Carlo calculations. This means that \( \frac{dE}{dS} \) is now a constant and can be taken out of the integral in Equation 60 to give

\[
\Delta = \sum \frac{1}{\varepsilon_e}(dE/dS)h(0) \int_0^{S''} \exp(S \cos \theta/\lambda_s) dS
\]  

(61)

where the integration is carried out over each individual step in a history and the summation is over the entire history.

Carrying out the integration in Equation 61 and substituting \( z \) for \( S \cos (\theta) \) one obtains

\[
\Delta = \sum \frac{1}{\varepsilon_e}(dE/dS)h(0)(\lambda_s/\cos \theta)[\exp(-z''/\lambda_s) - \exp(-z'/\lambda_s)]
\]  

(62)

where \( z'' \) and \( z' \) are depths of the incident electron at the beginning and end of a step. In order to exactly evaluate Equation 62 one needs to know the value of \( \varepsilon_e, h(0), \) and \( \lambda_s \). However, if the results of the secondary electron production calculations are expressed as ratios of secondary electron yields, then the constants \( \varepsilon_e \) and \( h(0) \) cancel out leaving only \( \lambda_s \) to determine. The value of \( \lambda_s \) can be experimentally determined and Seiler (59) has summarized various experi-
mentally determined values of $\lambda_s$. The choice of the exact value of $\lambda_s$ to be used in the calculations is discussed in a later section. Seiler also determined that the maximum depth of secondary electron production is approximately $5\lambda_s$. Therefore, the summation in Equation 62 need only be carried out over the part of the incident electron history that is within $5\lambda_s$ of the surface.

Computer programs that evaluate Equation 62 for histories of backscattering and incident electrons are given in Appendix A along with simplified flow diagrams. These programs calculate $\Delta$ and the user must calculate the ratios in order to eliminate the need to know $\varepsilon_e$ and $h(0)$. 

COMPUTATIONAL TECHNIQUES

The purpose of this study is to take the existing Monte Carlo method techniques and apply them to the problem of subsurface void contrast in the SEM. It is necessary to understand the role of subsurface void contrast in order to properly interpret micrographs of materials containing voids or bubbles. As was discussed previously, the two theories, single and multiple scattering, that can be used in the Monte Carlo method simulations each have advantages and disadvantages. To see which of these theories or a combination of these theories is best suited to the problem of subsurface void contrast let us consider the geometric model to be used in the simulation.

Figure 2 shows a cross section of the specimen model used in the calculations. The figure shows the void lying below the surface of the specimen with an electron beam incident to the specimen surface. Boundaries are shown at the maximum depth of secondary electron production, $5\lambda_s$, and at the maximum depth of the bottom of the subsurface voids. This latter boundary is arbitrary. Single scattering theory could be used to follow the electron trajectory through the entire specimen but this would be very time consuming. As mentioned previously single scattering theory need only be used when the fine details of the electron histories are
Figure 2. Cross section of the specimen model used in the computations
desired. This fine detail is required in the region of the specimen between the surface and the maximum depth of secondary electron production. This is because multiple scattering theory overestimates the mean free path of the incident electrons in this region and gives erroneous secondary electron production. This has been shown by Shimizu and Murata (29). The next region to consider is between the maximum depth of secondary electron production boundary and the maximum void depth boundary. In this region the subsurface voids are analyzed. In the calculations the maximum void depth boundary was set at 1200Å. We are interested in voids on the order of \((50Å)^3\) to \((1000Å)^3\) in volume because this range of void sizes is frequently found in radiation damaged material. As will be shown later the multiple scattering step length for the incident electrons is 1200Å. This means that the electron will only undergo one collision as it passes through the region where voids occur. Since the average step length of the incident electrons is 600Å, using multiple scattering theory many of the electrons would enter the top of the void without undergoing a collision. The use of multiple scattering theory, therefore, would bias the calculations towards the electrons entering the void with the initial direction of travel. To avoid this problem single scattering theory is used in this region of the specimen.

Below this region the specimen is assumed to be composed
of a solid homogeneous material. Here, we are not interested in the details of the electron histories and multiple scattering theory can be used in the simulation. Therefore, the Monte Carlo calculations that are used to analyze the effects of subsurface voids on the backscattered and secondary electron signals use single scattering theory when the electron is above the maximum depth of the bottom of the voids and multiple scattering theory when the electron is below this depth. This allows the simulation to use the detailed case history model of electron interactions with the specimen where it is necessary to know the details of the history but retain the computational speed of the condensed case history model when the details of the interactions are not needed. The algorithm for this Monte Carlo method program is discussed next.

Monte Carlo Method Computer Algorithm

Since the geometric model used in the simulations consists of two separate regions the calculations use two separate algorithms. The single scattering theory algorithm starts with the electrons at the surface of the specimen and follows them to the point where they backscatter, are absorbed, or cross the maximum void depth boundary. In the latter case the multiple scattering theory algorithm picks up the electron history and follows the electron until it is absorbed or until
it crosses back into the region above the maximum void depth boundary. In this last case the single scattering theory algorithm picks up the electron history and follows the electron until it is backscattered or absorbed, irrespective of the electrons position in the specimen.

The single scattering theory algorithm uses the screened Rutherford cross section to determine the polar scattering angle, the mean free path of the electron to determine the step length, and the Bethe continuous energy loss equation to determine the energy of the electron. The algorithm consists of a series of steps that are repeated throughout the history of the electron. The steps consist of the following series of calculations.

1. Initialize energy, $E_0$, position, $r_0$, and direction of travel $\bar{n}_0(\theta, \phi)$ of the electron.

2. Determine the distance the electron travels before undergoing an elastic collision.
   a. Set Equation 19 equal to a random number, $R_1$, and calculate the path length

$$\Delta S_n = -\ln(R_1) N\sigma(E_n)$$

where $N\sigma(E_n)$ is determined from Equation 23 using the expression for the differential scattering cross section from Equation 25

$$N\sigma(E_n) = \frac{(\pi N Z_e^2 e_A^4)}{[4E_n^2 \beta_s (1+\beta_s)]}.$$
This uniquely determines the path length, $\Delta S_n$, between elastic scattering events.

3. Determine the electron energy at the end of the step, $E_{n+1}$.
   a. Use the energy value at the start of the step, $E_n$, in the Bethe continuous energy loss equation, Equation 32, to determine $(\frac{dE}{ds})_n$.
   b. Determine $E_{n+1}$ using the equation

   $$ E_{n+1} = E_n - \Delta S_n (\frac{dE}{ds})_n. $$

4. Determine the new direction of electron travel.
   a. Determine the polar scattering angle, $\beta$.
      (1) Using the expression for $\sigma(E)$ (Equation 23) in Equation 24 and carrying out the integration one obtains

      $$ F_\beta(\beta) = \frac{(1+\beta_s)(1-\cos \beta)}{(1+\cos \beta+2\beta_s)} $$

      Setting $F_\beta(\beta)$ equal to a random number and solving for $\cos \beta$ one obtains

      $$ \cos \beta = 1 - (2\beta_s R_2)/(1+\beta_s R_2) $$

      where $R_2$ is a random number.
   b. Determine the azimuthal scattering angle, $\alpha$.
      Since $\alpha$ is assumed to be uniformly distributed between zero and $2\pi$

      $$ \alpha = R_3 2\pi $$

      where $R_3$ is a random number.
c. Compute $\theta_{n+1}$ and $\phi_{n+1}$ corresponding to $\beta$ and $\alpha$ using the geometric relationships in Equations 10, 11, and 12.

5. Check position and energy of the electron to see if the history is to be terminated. If history is not terminated return to Step 2. If the history is terminated return to Step 1.

A computer program using this single scattering model Monte Carlo method algorithm is given in Appendix A. A simplified flow diagram is also given in this appendix. The program is designed for simulation of the interaction between an electron beam and a thin specimen. The program includes the capability of recording the electron data at selected boundaries. The program is used to produce histories that are used in the calculation of the secondary electron production of the incident electrons.

The multiple scattering theory Monte Carlo algorithm uses the Goudsmit and Saunderson theory of scattering to determine the polar angle distribution, the Bethe continuous energy loss equation to determine the electron energy, and the constant number of elastic scattering events criterion to determine the step length. Because the integral probability function for the polar scattering angle, $\beta$, is determined by an expansion it cannot be directly solved for $\beta$. Therefore, it is necessary to generate a table of cross sections for
values of $\beta$ between zero and $\pi$ and use this table to determine the scattering angle. Since fixing the initial electron energy and number of elastic scattering collisions per multiple scattering step determines all the electron energies and all the step lengths a table of the electron energies and step lengths can also be constructed. Therefore, to execute the multiple scattering theory Monte Carlo algorithm it is necessary to have a computer program which produces the energy and step length for each multiple scattering step and the cross sectional information for each elastic scattering collision simulated by the multiple scattering theory. The following computer algorithm is used to compute these quantities assuming that the initial energy of the multiple scattering and the number of elastic scattering collisions per multiple scattering step have been chosen. The algorithm is composed of the following steps.

1. Determine $\Delta S_0$, the initial path length using Equation 54, and record $\Delta S_0$ and $E_0$, the initial energy, on magnetic tape.

2. Compute the desired number of step lengths, energies at the beginning and end of each step, and energy loss per unit path length for each step and record these quantities.
   a. Use the Bethe energy loss equation, Equation 32, to determine the energy loss for the $n_{th}$
b. Compute the energy at the end of the \( n_{th} \) step, \( E_{n+1} \), using the equation

\[ E_{n+1} = E_n - \Delta S_n \frac{dE}{dS}_n. \]

c. Compute the \( n+1 \) step length, \( \Delta S_{n+1} \), using Equation 54.

3. Compute the values of the polar angle integral probability function, \( F_m(\beta) \), for angles between zero and \( \pi \) for each collision using Equation 50.

4. Using the table of values of the integral probability function for the scattering angle \( \beta \) computed in step 3, compute \( N \) values of the angle \( \beta \) that correspond to \( N \) values of the probability function that are uniformly distributed between zero and one. Record this table of the scattering angle \( \beta \) for multiple scattering theory. Use an interpolation routine to determine the \( N \) values of \( \beta \) that correspond to the probability function values.

The computer program that uses this algorithm is given in Appendix A along with a simplified flow diagram.

A Monte Carlo method algorithm which uses this information can now be written to simulate the electron interactions with the specimen using the multiple scattering theory Monte Carlo method. The algorithm is composed of the
following steps.

1. Initialize the electron position, \( r_0 \), and direction of travel, \( \vec{n}_0 (\theta, \phi) \).

2. Retrieve from the magnetic tape the values of the path lengths, \( \Delta S_n \), the energies at the beginning and end of the step, \( E_n \) and \( E_{n+1} \), the energy loss per unit path length, \( (\frac{dE}{dS})_n \), and the scattering angles for the step.

3. Compute the path length the electron travels before the \( n_{\text{th}} \) elastic collision, \( \Delta S^*_n \), using the expression

\[
\Delta S^*_n = R_1 \Delta S_n,
\]

where \( R_1 \) is a random number.

4. Determine the angles of scattering, \( \theta \) and \( \phi \).
   
a. Generate random number \( R_2 \).
   
b. Using an interpolation routine find the value of the polar scattering angle, \( \beta \), that corresponds to a value of the integral probability function equal to \( R_2 \) for the \( n_{\text{th}} \) multiple scattering elastic collision.
   
c. Determine the azimuthal scattering angle, \( \alpha \), where \( \alpha \) is given by

\[
\alpha = R_3 \cdot 2\pi
\]

and \( R_3 \) is a random number.
d. Compute $\theta_{n+1}$ and $\phi_{n+1}$ which correspond to the angles $\beta$ and $\alpha$ using the geometric relationships given in Equations 10, 11, and 12.

5. Let the electron travel the remainder of the multiple scattering path length, $\Delta S^{**}$, where

$$\Delta S^{**} = S_n - S^*_n.$$ 

6. Check position and energy of the electron to see if the history can be terminated.

7. Continue steps 2 through 6 until the table of electron energies and step lengths is exhausted and then terminate the history.

The combined single and multiple scattering theory Monte Carlo method algorithm is used in the simulation of the interactions between the electron and the specimen. The single scattering theory is used where a detailed case history is required and the multiple scattering theory is used where only a condensed case history is required. The electrons that emerge from the boundary at the maximum void depth have a variety of energies. Therefore, it is necessary to follow the electron using single scattering theory until the electron reaches one of the stored multiple scattering theory energies. It is also necessary to select the initial multiple scattering energy and this choice is discussed later. For the present it is assumed that the energy has been chosen. The combined single and multiple scattering theory Monte Carlo method
algorithm uses the details of the single and multiple scattering algorithms previously given and is outlined in the following steps.

1. Select the incident electron energy, $E_0$, position $r_0$, and direction $\vec{n}_0(\theta, \phi)$.
2. Use single scattering theory until the electron crosses the maximum void depth boundary and record the electron history.
3. Find the recorded multiple scattering energy that is less than the electron's energy at the maximum void depth boundary.
4. Continue using single scattering theory until the electron energy is less than this multiple scattering energy.
5. Compute the electron position that corresponds to the multiple scattering energy.
6. Use multiple scattering theory until the electron is absorbed or until it crosses the maximum void depth boundary.
7. If the electron crosses the maximum void depth boundary continue the electron history using the single scattering algorithm until the electron is absorbed or crosses the surface.

In the single scattering theory portion of the program the electron is considered absorbed when its energy is equal
to two percent of the incident electron energy. In the multiple scattering theory section of the program the electron is considered absorbed when all the stored multiple scattering steps have been used or the remaining multiple scattering path length is less than the distance between the electron position and the surface. The program which utilizes this algorithm is given in Appendix A along with a simplified flow diagram. This program produces the electron histories that are used by the secondary production of backscattered electron program and the void analysis program.

Subsurface Void Analysis Computer Algorithm

In order to better understand the problem of subsurface void analysis consider the geometry of the problem to be simulated by the program shown in Figure 3. A parallelepiped void is situated a certain depth below the surface of the specimen. The void has a specific width, length, and thickness. The electron beam is incident at the origin of the coordinate system. Figure 4 shows some of the possible electron histories in a specimen containing a parallelepiped void. History 1 shows an electron that passes through a void when the electron is headed away from the specimen surface. Histories 2 and 5 show electron trajectories that have passed through the void when the electron is headed both towards and
Figure 3. Geometry used in the analysis of subsurface voids.
Figure 4. Possible electron histories in a specimen containing a void
away from the specimen surface. History 2 shows the case when the distance the electron travels inside the void is the same in both directions. In history 5 the electron travels a greater distance inside the void when the electron is headed away from the surface than when it is headed towards the surface. History 3 shows an electron that backscatters at a shallower depth than the top of the void and history 4 shows an electron that misses the void even though it starts towards the surface at a depth greater than the top of the void.

In the analysis of subsurface void contrast we are interested in the difference between the backscattering and secondary electron coefficients of the solid specimen and the specimen containing a void. When an electron travels through a void it travels a direct path because the probability of an electron suffering a collision inside the void is zero. Also the electron enters and leaves the void with exactly the same energy since no inelastic collisions occur inside the void. This means that the passage of an electron through a void only changes the position of the electron. Therefore, if an electron goes through an identical set of elastic collision and energy losses in a solid specimen and in a specimen containing a void the only difference between the histories is the final position of the electron. This is illustrated in Figure 5. At the end point of history 1A the electron has
Figure 5. Electron histories with the same number of elastic collisions and path lengths between collisions in a solid specimen and a specimen containing a void.
exactly the same energy and direction of travel as the back-scattered electron of history 1. The same is true for the absorbed electron of histories 2A and 2. The only difference between the electron histories in a specimen with a void and those in a solid specimen is the final position of the history. However, the final position of the electron history 1A shown in Figure 5 is not a termination point because the electron has sufficient energy to continue the history. Therefore, this electron history must be continued to determine the fate of the electron. Since the electron shown in history 1A must travel through more material in order to escape from the specimen than the electron in history 1, the probability of backscattering and the secondary electron production of the two histories is not the same. In the case of history 2A the electron has been absorbed at a different position than the absorption of the electron in history 2 but this has no effect on the backscattering or secondary electron yield of the specimens. Therefore, it is possible to calculate the difference between the backscattering and secondary electron coefficients of the solid specimen and the specimen containing a void by only considering the backscattered electron histories.

It would be possible to calculate the backscattering and secondary electron coefficients of a specimen containing a void by analyzing each void geometry with a different set of
Monte Carlo calculations but it has just been demonstrated that the histories of electrons in a solid specimen and in a specimen containing a void are identical, except for position, up to a point. Therefore, if we have recorded electron histories from a solid specimen we can calculate the point at which the electron trajectory would enter a void and the path length the electron travels inside the void. By computing the change in coordinates due to traveling the path length inside the void, the new end position of the recorded electron history can be determined and the fate of the electron can be computed by continuing the electron history using Monte Carlo calculations.

In order to analyze the effect of various size subsurface voids on the backscattering and secondary electron coefficients of a specimen it is necessary to record backscattered electron trajectories in a solid specimen. Since we have arbitrarily set a lower boundary below which no voids occur, it is only necessary to record the electron histories between the surface of the specimen and this arbitrary boundary. This is because changes in the histories only occur when the electron passes through a void and the change is constant throughout the rest of the history. Since the electron can enter the top or bottom of a void it is necessary to record the electron's position, direction of travel, and energy at this point. Therefore, the combined theory Monte Carlo
program records the electron parameters at boundaries which correspond to the tops and bottoms of the voids.

As a result of this discussion a series of programs need to be used to determine the effect of subsurface voids on backscatter and secondary electron coefficients. The combined theory Monte Carlo method program is needed to record the backscattered electron histories in the region where the voids are going to be inserted and to calculate the backscattering electron coefficient of the solid specimen. These histories can be used by the programs to calculate the secondary electron coefficient for the primary and backscattered electrons. These histories can then be used by a program which analyzes the effect of various sized voids on the histories and the changes in the backscattering and secondary electron coefficients.

The subsurface void analysis program is used to calculate the secondary and backscattering coefficients for a specimen containing a void. This program analyzes the backscattered electron histories produced by the combined theory program to determine if the electron enters the void and what path length the electron travels inside the void. The subsurface void analysis program determines where the recorded history terminates after the passage through the void has been calculated. If the end point of the electron history is now inside the specimen, the single scattering theory Monte Carlo
Carlo method calculations are used to determine if the electron is again backscattered or if it is absorbed. The program computes the new number of backscattered electrons. As noted in the description of Figure 4, some of the recorded backscattering electron histories do not enter the void. Therefore, the fate of the electron is unchanged for the case of a specimen containing a void, and the secondary electron production of the incident electron is unchanged. In order to compute the secondary coefficient for the specimen containing the void, it is necessary to know the secondary production of these "unchanged" histories. To do this the secondary production of each backscattered electron, that is the number of secondary electrons produced when the electron passes through the secondary electron production region of the specimen when it is headed towards the surface, is recorded on magnetic tape for use by this program. The program reads the secondary electron yield of backscattered electron histories that are unchanged in the specimen containing the void. This is added to secondary production of backscattered electron histories that are changed due to the void. This gives a new secondary electron yield due to the backscattered electrons. This program is given in Appendix A along with a simplified flow diagram. Appendix A also gives the necessary instructions for the proper execution of the various programs that are
needed to analyze the effects of subsurface voids on the backscattering and secondary electron coefficients.
RESULTS AND DISCUSSION

Cases Used to Test the Validity of the
Monte Carlo Method Computer Programs

The programs developed for this study were tested to check their validity. The results of the programs were compared to previous experimental and calculational results. Table 1 summarizes the tests performed to check these programs.

Table 1. Testing of programs used for the analysis of subsurface void contrast

<table>
<thead>
<tr>
<th>Program</th>
<th>Test</th>
</tr>
</thead>
<tbody>
<tr>
<td>Single scattering theory Monte Carlo method program</td>
<td>Comparison of angular distribution of transmitted electrons with experimental data</td>
</tr>
<tr>
<td>Multiple scattering data program</td>
<td>Comparison of angular distribution of transmitted electrons from a thin specimen with single scattering Monte Carlo calculations data for the same specimen</td>
</tr>
<tr>
<td>Combined single and multiple scattering theory Monte Carlo method program</td>
<td>Comparison of calculated backscattering coefficient with experimental data and previous calculations for a copper specimen with 20 keV incident electrons</td>
</tr>
<tr>
<td>Secondary electron production programs using trajectories produced by the combined theory Monte Carlo method program</td>
<td>Comparison of secondary coefficient for a copper specimen with 20 keV incident electrons and comparison with previously calculated secondary electron production parameters using a single scattering theory Monte Carlo program</td>
</tr>
</tbody>
</table>
The first program tested was the single scattering theory Monte Carlo method program. The program was tested by comparing the calculated angular distribution of electrons emerging from a thin copper specimen for the case of 20 keV electrons incident on the specimen at an angle of 90 degrees with experimental distributions. This program was tested using two different expressions of the screening angle, $\beta_s$, for use in the Rutherford cross section because previous Monte Carlo calculations have used different expressions for $\beta_s$. Three different equations for $\beta_s$ have been used in previous Monte Carlo calculations of electron interactions with solids. Shimizu, Murata, et al. (25, 27, 28, 29, 30, 31, 36, 37, 38) used Nigam's et al. (48) expression for $\beta_s$ in their calculations while McDonald et al. (35) used Mott and Massey's (44) expression for $\beta_s$ in their calculations. Bishop (32) used Wentzel's expression (46) in his calculations. All these expressions can be reduced to functions of $Z$ and $E$ only as shown in Equations 26b, 27b, and 29b. Since the constant in the equation for $\beta_s$ using Wentzel's expression is between those of Nigam et al. and Mott and Massey it was decided to test the latter two expressions first. In order to determine which of these expressions to use in the calculations and to check the validity of the program, calculations were performed which determined the probability of electron emergence from a thin copper specimen as a function
of the emergence angle. Cosslett and Thomas (55) have published experimentally determined curves of this probability for thin films of copper with 20 keV incident electrons. The Monte Carlo calculations were performed for the same thickness films. Figures 6, 7, 8, 9, and 10 show a comparison between the experimental curve and calculated values of the probability of emergence using the Nigam et al. and Mott and Massey expressions for $\beta_s$. For the 215 Å thick film (Figure 6), the comparison shows that the most probable angle of emergence calculated using the Nigam et al. expression for $\beta_s$ more closely agrees with the experimental value than the calculations using the Mott and Massey expression and the overall agreement between the theoretical and experimental curves is best for calculations using the Nigam et al. value of $\beta_s$. The same general conclusions hold for the 428 Å thick specimen calculational results shown in Figure 7. The calculations using the Nigam et al. $\beta_s$ value again show a value of the most probable emergence angle that compares favorably with the experimental value; however, the value of the cross section term is higher for the theoretical than experimental case. In the 656 Å thick film case, shown in Figure 8, neither theoretical curve shows good agreement with the experimentally determined most probable angle of emergence but the calculations using the Nigam et al. value come closer to the experimental most probable angle of emergence, and this
Figure 6. Angular distribution of electrons emerging from a 215 Å thick copper specimen with incident electron energy of 20 keV. Calculations were performed for 3000 incident electrons.
Figure 7. Angular distribution of electrons emerging from a 428 Å thick copper specimen with incident electron energy of 20 keV. Calculations were performed for 3000 incident electrons.
Figure 8. Angular distribution of electrons emerging from a 656 Å thick copper specimen with incident electron energy of 20 keV. Calculations were performed for 3000 incident electrons
Figure 9. Angular distribution of electrons emerging from a 897 Å thick copper specimen with incident electron energy of 20 keV. Calculations were performed for 3000 incident electrons.
Figure 10. Angular distribution of electrons emerging from a 1395 Å thick copper specimen with incident electron energy of 20 keV. Calculations were performed for 3000 incident electrons.
Theoretical curve has the same general shape as the experimental curve. Figure 9 shows the comparison for a 897 Å thick film. In this case the calculated curve using the Nigam et al. expression is close to the experimental curve while the curve calculated using the Mott and Massey expression significantly deviates from the experimental curve. Again the most probable angle of emergence predicted by the calculations using the Nigam et al. expression agrees with the experimental curve. The theoretical curve that was calculated using the Nigam et al. expression for $\beta_s$ also more closely agrees with the experimental curve than the curve obtained using the Mott and Massey expression in the calculations for the 1395 Å thick specimen as shown in Figure 10.

Based on this discussion it can be seen that the calculations using the Nigam et al. expression for $\beta_s$ more closely agree with the experimental curves. This is true both for the prediction of the most probable angle of emergence and the overall agreement between the theoretical and experimental curves. Therefore, the single scattering theory Monte Carlo calculations, using the Nigam et al. expression for $\beta_s$ in the screened Rutherford cross section, give results that favorably compare with the experimental curves. Based on these comparisons it was decided to use the Nigam et al. expression for $\beta_s$ in all the calculations using the screened Rutherford cross section.
The next program tested was the multiple scattering data program. This program was tested by comparing the angular distribution of electrons emerging from a thin specimen calculated by the multiple scattering angular cross section equation, used in this program, with the angular distribution of electrons emerging from a thin specimen calculated by the single scattering theory Monte Carlo program. The criterion for the comparison is that the multiple scattering theory should give electron angular distributions that favorably compare with the distributions calculated by the single scattering theory Monte Carlo program. The multiple scattering theory data program produces the angular distribution of electrons traveling a specific step length. The single scattering theory Monte Carlo calculations produce the angular distribution of electrons emerging from a thin specimen of a given thickness. The path length traveled by the electron through the thin specimen can be calculated by dividing the specimen thickness by the cosine of the most probable angle of emergence. Since the angle of emergence from thin specimens is small, the approximation was made that the path length traveled by the electron in the specimen was equal to the thickness of the specimen. Using this approximation it is possible to make a direct comparison between the multiple scattering theory angular cross section for a specific step length, (which is the probability of an electron emerging at
an angle after traveling this step length), and the distribution of electrons emerging from a thin specimen, as calculated by the single scattering theory Monte Carlo method program.

The expansion used to compute the multiple scattering theory angular cross section for a specific step length is given by Equation 48. In the computer program the summation was continued until the difference between successive terms in the expansion was less than 0.0001. By analyzing the calculations it was determined that the expansion converged to the desired degree of accuracy in 40 or 50 terms. In order to conserve the amount of computer core space required to store the values of the Legendre polynomials used in the expansion, it was decided to set an upper limit of 56 on the number of terms used in the expansion.

The comparison of the emerging electron distributions was done for 897 Å, 1100 Å, 1200 Å, and 1395 Å thick copper specimens for 20 keV incident electrons. The comparisons are shown in Figures 11, 12, 13, and 14. Based on these figures the agreement between the calculations using single scattering theory and those using multiple scattering theory is good for the 897 Å, 1100 Å, and 1200 Å thick specimens. The case of the 1395 Å thick copper specimen shows a discrepancy between the two theories. This discrepancy is thought to be due to the inapplicability of multiple
Figure 11. Angular distribution of electrons emerging from a 897 Å thick copper specimen with incident electron energy of 20 keV.
Figure 12. Angular distribution of electrons emerging from a 1100 Å thick copper specimen with incident electron energy of 20 keV.
Figure 13. Angular distribution of electrons emerging from a 1200 Å thick copper specimen with incident electron energy of 20 keV
Figure 14. Angular distribution of electrons emerging from a 1395 Å thick copper specimen with incident electron energy of 20 keV
scattering theory for this length of step in copper at this energy.

Since the multiple scattering theory Monte Carlo calculations use the approximation that the number of scattering collisions is constant in each multiple scattering theory step, it is necessary to choose a value of \( p_e \), the number of scattering collisions per multiple scattering step. The choice is made by comparing the angular distribution of electrons emerging from thin films as calculated by single and multiple scattering theory as shown in Figures 11, 12, and 13. The 1395 Å case is not considered because of the discrepancy between single and multiple scattering theory. Since \( p_e \) is directly related to the path length traveled by the electron, it is desirable to choose the longest possible path length for a given specimen and energy, so that the fewest possible multiple scattering steps are used in the calculations. Since the longest step length that gives good agreement between single and multiple scattering is 1200 Å, this step length was chosen for a copper specimen with 20 keV incident electrons. Using this value of \( \Delta S_n \) in Equation 54 one obtains a value of \( p_e \) equal to 22.6. This agrees with Cosslett and Thomas' (55) experimentally determined value of \( p_e \) equal to 25 ± 5 for copper.

The next program tested was the combined single and multiple scattering theory Monte Carlo calculations program.
However, before this program can be executed the specimen, incident electron energy, incident beam angle, maximum depth for the bottom of the voids, initial energy of multiple scattering, and number of multiple scattering steps must be chosen. Since good agreement between experimental and calculational results had been obtained for the problem of 20 keV electrons interacting with a copper specimen, it was decided that the calculations analyzing the contrast effects of subsurface voids should be done on an infinitely thick copper specimen with a 20 keV electron beam incident on the specimen surface at an angle of 90 degrees. Therefore, this program was tested for a copper specimen with 20 keV incident electrons.

Since we are interested in analyzing the contrast effects of voids that are close to the surface it was decided that the maximum depth of the bottom of the voids would be 1200 Å. Therefore, single scattering theory calculations only need to be carried out to this depth and after the electron crosses this boundary multiple scattering calculations can be used. As explained in the Computational Techniques section, the electrons emerge from this boundary with a variety of energies and a choice must be made for the initial electron energy for multiple scattering. There are two opposing criteria that are used to select this energy. The initial
multiple scattering energy should be low enough that a significant portion of the emerging electrons have energies higher than the initial multiple scattering energy. But, the initial multiple scattering energy should be high enough that the program has to perform few single scattering calculations in order to lower the incident electron's energy to the initial multiple scattering theory energy. Figure 15 shows a graph of the fraction of electrons emerging from a 1200 Å thick copper specimen with less than a certain energy versus the emergence energy. The graph results from calculations for 3000 incident electrons. The electrons emerge with a maximum energy of 19.1 keV and a minimum energy of 4.7 keV. An initial multiple scattering energy of 18.9 keV was chosen because 60% of the electrons have energy greater than 18.9 keV and the electrons that emerge with the maximum energy must travel about six mean free path lengths to reach this energy. This choice is a reasonable compromise between the two criteria that have to be considered when choosing the initial multiple scattering energy.

The number of multiple scattering steps is determined by the energy at which the electron history is terminated. In these calculations it was desired to follow the electrons to 2% of their incident energy. In order to do this 25 multiple scattering steps were chosen.

Besides the comparison of backscattering electron...
Figure 15. Integral energy distribution curve for electrons transmitted through a 1200 Å thick copper specimen. The incident electron energy is 20 keV.
coefficients another test of this program is the accuracy of the secondary electron parameters that are calculated using the electron histories produced by the combined single and multiple scattering theory Monte Carlo method program. However, it is necessary to choose some constants to be used in secondary electron production calculations before these calculations can be performed.

As discussed in the Theoretical Development section the only parameter that needs to be chosen to calculate the secondary electron coefficient ratios is $\lambda_s$, the mean free path of secondary electrons, because of the ratioing of the secondary electron coefficients. Seiler (59) reports two values of $\lambda_s$ for copper. One is 5 Å and the other is 20 to 24 Å. To determine which one of these values to use in the calculations the secondary electron coefficient calculated using a value of $\lambda_s$ for copper with 20 keV incident electrons should correspond favorably to the experimental value. No experimental value could be found for $\delta$ of copper at 20 keV. Therefore, it was necessary to interpolate existing data for copper. Wittry (60) determined values of $\delta = .119$ at 30 keV and $\delta = .390$ at 5 keV for a copper specimen. In order to interpolate for the 20 keV case it is necessary to know the relationship between the secondary electron coefficient and the energy of the incident electrons. Kanter (61) found that the relationship between the secondary electron coefficient and
electron energy is similar to the Bethe energy loss law and that the shape of the secondary electron coefficient versus energy curve is the same as the Bethe energy loss law for incident electron energies between 5 and 20 keV for an aluminum specimen. Since the slope of the secondary coefficient curve is the same as the Bethe continuous energy loss curve we will assume that

\[
\frac{\delta(20 \text{ keV})}{\delta(5 \text{ keV})} = \frac{dE/dS(20 \text{ keV})}{dE/dS(5 \text{ keV})}
\]

where \(\delta(5 \text{ keV})\) is known from Wittry's data and \(dE/dS\) at 20 and 5 keV can be calculated using Equation 32. By using this expression one obtains a value of \(\delta\) for copper at 20 keV of 0.147.

To calculate \(\delta\) for copper using the secondary electron production program, where \(\delta\) is \(\Delta\) divided by the number of incident electrons, it is necessary to know \(\lambda_s\), \(\epsilon_e\), and \(h(0)\) since the secondary electron coefficient is not ratioed with another coefficient to cancel out the effect of \(\epsilon_e\) and \(h(0)\). \(h(0)\) can be assumed to be a constant for all materials and energies so that it is only necessary to know the value of \(\lambda_s\) and \(\epsilon_e/h(0)\) in order to calculate \(\delta\). Dekker (62) has calculated values of \(\epsilon_e/h(0)\) for metals using experimental values of \(\lambda_s\) and \(\delta\). Dekker determined that values of \(\epsilon_e/h(0)\) of 150 to 160 eV gave calculated values of \(\delta\) that corresponded to experimental values of \(\delta\) for metals using the
theory of Bruining and Salow. This corresponds to the findings of Simon and Williams (63) for the value of $e_e/h(0)$. Using a value of $e_e/h(0)$ of 160 eV, calculations were performed to obtain the secondary electron coefficient using the values of $\lambda_s$. The results are shown in Table 2.

Table 2. Secondary electron coefficients calculated for a copper specimen with a 20 keV perpendicularly incident beam

<table>
<thead>
<tr>
<th>$\lambda_s$ (Å)</th>
<th>$e_e/h(0)$ (eV)</th>
<th>$\delta$</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>160</td>
<td>0.036</td>
</tr>
<tr>
<td>20</td>
<td>160</td>
<td>0.152</td>
</tr>
<tr>
<td>24</td>
<td>160</td>
<td>0.171</td>
</tr>
</tbody>
</table>

The closest calculated value to the experimental value of $\delta = 0.147$ is for the case of $\lambda_s = 20$ Å. Because of this, the value of $\lambda_s$ used in the calculations was 20 Å.

Using the combined single and multiple scattering theory program and the programs to calculate the secondary electron production of the incident and backscattered electrons, backscattering and secondary electron coefficients were obtained for a solid copper specimen with 20 keV incident electrons. These calculated values are shown in Table 3 along with previously calculated values and experimental values of these parameters. $\delta^*$ is the number of secondary electrons.
produced by a single backscattering electron divided by the number of secondary electrons produced by a single incident electron.

Table 3. Comparison of present calculations with previous calculations and experimental results, $\beta^* = (\delta_n/\eta)/\delta_p$

<table>
<thead>
<tr>
<th>Source</th>
<th>Backscattering Coefficient</th>
<th>Proportion of secondaries from backscattered electrons $\delta_n/\delta$</th>
<th>Secondary emission parameter $\beta^*$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Present Calculations</td>
<td>0.268</td>
<td>0.38</td>
<td>2.3</td>
</tr>
<tr>
<td>Murata (38) (calculational results)</td>
<td>0.314</td>
<td>0.43</td>
<td>2.4</td>
</tr>
<tr>
<td>Cosslett and Thomas (64) (experimental results)</td>
<td>0.290</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Heinrich (65) (experimental results)</td>
<td>0.309</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The present calculated value of $\eta$ appears to be a low but it differs from Cosslett and Thomas' experimental value by about the same amount as does Murata's value. Of the two experimental values it is felt that the Cosslett and Thomas value is probably better because of the exacting experimental technique used in their measurements. The $\delta_n/\delta$ values disagree by about the same magnitude as do the calculational $\eta$ values. This discrepancy is probably due to the difference in the
calculated values of $\eta$. The $\beta^*$ values are reasonably close to one another. This combined model Monte Carlo method program gives precise results for a copper specimen with 20 keV incident electrons and can be used to examine the effects of subsurface voids on the secondary and backscattering coefficients.

The combined single and multiple scattering Monte Carlo method program requires approximately $50.00 of Central Processing Unit time to calculate 9,000 incident electron histories on the Iowa State University IBM360-65 computer. This cost compares favorably with comments by Kyser (66) of IBM who has been using some of the computer programs devised by Shimizu, Murata, et al. (29 and 36).

Calculation of Subsurface Void Contrast

The analysis of subsurface void contrast is done by computing the ratio between the backscattering electron coefficient for a specimen containing a void and the backscattering electron coefficient for the solid specimen. A similar ratio is computed between the secondary electron coefficient of a specimen containing a void and the solid specimen. These ratios are the theoretical contrast between a solid portion of a specimen and a portion of the specimen containing a subsurface void. The analysis is carried out using
the subsurface void analysis program. This program computes the number of backscattering and secondary electrons for given void size and depth using the recorded backscattering electron histories and the recorded secondary electron yield of the backscattering electrons.

As mentioned in the Computational Techniques section, it is necessary to choose boundaries which correspond to the tops and bottoms of the voids and have the combined theory Monte Carlo program record the electron's position, direction of travel, energy, and rate of energy loss at these boundaries. In actual specimens, voids are found in a variety of shapes and sizes. The shapes range from pyramids to spheres and the sizes range from about 10 Å in diameter to several thousand angstroms in diameter. For the purposes of this study the void shape considered is a parallelepiped with one face parallel to the surface. This shape was used because of its calculational simplicity. The minimum size void to be considered is a cubic void 50 Å on a side because this represents the practical resolution limit of the SEM. The minimum void depth considered is 50 Å because this allows calculations to be done in the secondary production region of the specimen. The maximum depth at which the bottom of a void can be located has been previously set at 1200 Å. The maximum void size considered in the calculations is a cubic void, 1000 Å on a side. Voids were analyzed at depths of 50 Å, 100 Å, 200 Å,
500 Å, 700 Å, and 900 Å. The edge sizes of the cubic voids considered were 50 Å, 100 Å, 200 Å, 300 Å, 400 Å, 500 Å, 600 Å, and 1000 Å. The thicknesses of other parallelepiped voids were 50 Å, 100 Å, 150 Å, 200 Å, 300 Å, 450 Å, 500 Å, and 650 Å. These cases should give an idea of the effect of changing the geometry of the void on the calculated contrast. In order to handle these voids, and other possible void geometries, boundaries were chosen at 50 Å, 100 Å, 200 Å, 300 Å, 400 Å, 500 Å, 600 Å, 700 Å, 800 Å, 900 Å, 1000 Å, 1100 Å, 1150 Å, and 1200 Å. These boundaries were also chosen so that identical size voids could be analyzed at different depths.

The first step in the analysis was to determine the precision of the calculations and to determine the number of electron histories that would have to be analyzed in order to have confidence in a single calculation of a given void geometry. The case chosen to check the precision of the void analysis program was cubic voids of 100 Å, 200 Å, 300 Å, 400 Å, 500 Å, and 600 Å edge size at a depth of 100 Å. The calculations were performed on 805 backscattering electron histories resulting from 3000 incident electrons.

Figure 16 shows the results of five calculations of the void analysis program for each size void using different random numbers to determine the fate of the recorded electron histories that terminate within the sample. The points on the
Figure 16. Secondary and backscattering coefficient ratios for a specimen containing a void. The cubic voids are at a depth of 100 Å. Each point represents the mean of five calculations using 3000 incident electrons.
graph represent the means of the five calculations and the error bars represent one standard deviation. The error in the backscattering coefficient ratios is on the order of $\pm 2\%$ for voids larger than $(200 \text{ Å})^3$, and the backscattering coefficient steadily decreases with increasing void size. The case of the secondary coefficient ratios is not as good. The smallest error bars, for the $(100 \text{ Å})^3$ case, represent a $\pm 2\%$ error while the $(600 \text{ Å})^3$ case has error bars of $\pm 8\%$. The error in the secondary coefficient ratios tends to increase as the size of the void increases. This is due to the fact that fewer electrons enter the secondary electron production region as the void size increases and the variation in secondary electron production of each backscattered electron has more effect on the secondary electron coefficient as the number of backscattered electrons decreases. Figure 16 does show a significant peak in the secondary coefficient ratio. This number of histories does give adequate precision for the backscattering coefficient ratios; however, the use of the single calculations of the secondary electron coefficient ratios for large voids is imprecise because of the large error associated with these measurements.

To improve the precision of the calculations 9000 incident electrons were used to obtain recorded histories of more backscattered electrons. The coefficients calculated for
the solid specimen were the same as those shown in Table 3. The 2409 backscattered electron histories were then used in the void analysis program to determine the effect of the cubic voids at a depth of 100 Å with the same void sizes as those shown in Figure 16. Figure 17 shows the results of five calculations for each void size. Again the points represent the means of the five calculations and the error bars represent one standard deviation. Figure 17 shows the increased precision of the calculations for both the secondary and backscattering electron coefficient ratios using the larger number of histories. There is about a ± 2% error in the secondary coefficient ratios and a ± 1% error in the backscattering coefficient ratios of the various sized voids considered. The trend of a steadily decreasing backscattering electron coefficient ratio as the void size increases is again seen. The peak in the secondary electron coefficient ratio at (200 Å)³ is also observed with the ratio steadily decreasing for larger voids. The precision of the secondary electron coefficient ratios is greatly increased for the large voids as compared to the 3000 incident electron case. Since the error is independent of void size and depth it is felt that the error can be attributed to the random number distribution. Based on this analysis of the error of these calculations single subsurface void analysis computations using the 2409 backscattered electron histories can be used
Figure 17. Secondary and backscattering coefficient ratios for a specimen containing a void. The cubic voids are at a depth of 100 Å. Each point represents the mean of five calculations using 9000 incident electrons.
to analyze the trends of the electron coefficient ratios as a function of the void geometry.

The void analysis program utilized in these calculations uses the approximation that the backscattered electrons only enter the top and the bottom of the void. This approximation was made for two reasons. Since the voids are close to the surface of the specimen and the mean free path of 20 keV electrons is 80 Å, it was assumed that almost all of the electrons would enter the top of the void. Secondly, since the exit area of the backscattered electrons is enclosed in a one micron diameter circle and the most probable energy of the backscattered electron spectrum is about 17 keV, the probability of an electron entering the void is small and the probability of entering the side of the void is even smaller.

To check this approximation the void analysis program shown in Appendix A was written to check for the side entry of the electrons. In the cases considered so far, the void with the highest probability of an electron entering through the side is the (600 Å)³ void. A comparison between the results of the two programs is given in Table 4.

The standard deviations for both analyses overlap in both the backscattering and the secondary electron coefficient ratio cases. The fact that the means of the analyses using the side entry routine are lower than the means of the analyses neglecting the side entry is thought to be a function
Table 4. Comparison of the results of void analysis programs that consider and do not consider electron entry through the side of the void. Calculations are for a (600 Å)³ void at a depth of 100 Å

<table>
<thead>
<tr>
<th>Type of analysis</th>
<th>Mean (δ void/δ solid)</th>
<th>σ (δ void/δ solid)</th>
<th>Mean (η void/η solid)</th>
<th>σ (η void/η solid)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Side entry analyzed</td>
<td>0.993</td>
<td>0.015</td>
<td>0.783</td>
<td>0.019</td>
</tr>
<tr>
<td>Side entry not analyzed</td>
<td>1.008</td>
<td>0.015</td>
<td>0.814</td>
<td>0.012</td>
</tr>
</tbody>
</table>

Based on three calculations.

Based on five calculations.

of the random numbers because the inclusion of side entries should decrease the average path length traveled by the electrons toward the surface. This makes the backscattering coefficient ratio for the program considering side entries greater than the ratio calculated by the program neglecting side entries. This effect should occur because most of the electrons enter the top of the void since the void has a large cross sectional area compared to the area of the electron distribution near the surface of the specimen and there is no difference between the two programs. However, the number of electrons that enter the void when they are headed toward the surface should be greater in the program that includes side entry than in the one that neglects it.
Therefore, some of the electrons should have a shorter path to the surface in the side entry program than in the program neglecting side entry and one would expect the backscattering coefficient ratio to be higher. Since no difference between the calculations using only top and bottom entry into the void and the calculations using side entry is observed it can be assumed that the approximation neglecting electrons entering the side of the void is valid for voids of 600 Å thickness or less. The approximation may be valid for thicker voids; however, since the probability of the electron crossing the side of the void increases with increasing void thickness, the void analysis program that considers side entry is used for voids thicker than 600 Å.

To see if the trends found in Figure 17 for 100 Å deep cubic voids continue for larger voids, calculations were run for a (1000 Å)³ void. The results are shown in Figure 18 along with the previous calculations. The trends are continued with both the backscattering electron coefficient and secondary electron coefficient ratios. Both ratios have lower values for the larger void.

The most thorough analysis was carried out for the cubic voids at a depth of 100 Å. However, more void geometries were analyzed using single calculations of the 2409 backscattered electron histories. Table 5 shows the results of calculations for voids at a depth of 50 Å. The
Figure 18. Secondary and backscattering coefficient ratios for a specimen containing a cubic void at a depth of 100 Å. Each point represents the mean of five calculations using 9000 incident electrons except for the (1000)^3 case where four calculations using 9000 incident electrons were used to compute the mean.
one significant difference in the calculations at a depth of 50 Å is that the void is in the secondary electron production region. For the purposes of this analysis the $\delta_p$ for the configuration was assumed to be the same as the $\delta_p$ for a 50 Å thick film of copper. This assumption is made because the mean free path of the 20 keV electron in copper is 80 Å and almost all of the electrons will enter the top of the void terminating their secondary production at a depth of 50 Å.

Table 5. Ratios of secondary and backscattering electron coefficients for parallelepiped voids at a depth of 50 Å

<table>
<thead>
<tr>
<th>Void thickness Å</th>
<th>Void length Å</th>
<th>Void width Å</th>
<th>$\eta_{void} / \eta_{solid}$</th>
<th>$\delta_{void} / \delta_{solid}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>50</td>
<td>50</td>
<td>50</td>
<td>0.97</td>
<td>1.00</td>
</tr>
<tr>
<td>150</td>
<td>50</td>
<td>50</td>
<td>0.95</td>
<td>1.04</td>
</tr>
<tr>
<td>650</td>
<td>50</td>
<td>50</td>
<td>0.83</td>
<td>0.98</td>
</tr>
<tr>
<td>50</td>
<td>100</td>
<td>100</td>
<td>0.97</td>
<td>1.01</td>
</tr>
<tr>
<td>150</td>
<td>100</td>
<td>100</td>
<td>0.92</td>
<td>1.05</td>
</tr>
<tr>
<td>450</td>
<td>100</td>
<td>100</td>
<td>0.88</td>
<td>1.02</td>
</tr>
<tr>
<td>650</td>
<td>100</td>
<td>100</td>
<td>0.84</td>
<td>0.99</td>
</tr>
<tr>
<td>150</td>
<td>900</td>
<td>900</td>
<td>0.94</td>
<td>1.04</td>
</tr>
</tbody>
</table>
For voids with a 50 Å by 50 Å cross section the backscattering electron coefficient ratio steadily decreases with increasing void thickness and the secondary electron coefficient ratio has a peak at a thickness of 150 Å and then decreases. The same trend is seen for the voids with a 100 Å by 100 Å cross section. These trends can be explained by the fact that at a depth of 50 Å the incident electron pattern is extremely dense while the backscattering pattern is diffuse. Therefore, almost all electrons enter the void when they are headed away from the specimen surface but miss the void when they are headed towards the surface.

An analysis was next carried out at a depth of 200 Å. The results of the analysis are shown in Figure 19 for cubic voids of 100 Å, 200 Å, 300 Å, and 400 Å edge sizes. The same basic pattern of coefficient ratios is observed. The backscattering electron coefficient steadily decreases with increasing void size while the secondary electron coefficient ratio reaches a peak and then decreases.

Table 6 shows the results of an analysis carried out at depths of 500 Å, 700 Å, and 900 Å. Again the same basic pattern of the secondary and backscattering electron coefficient ratios as a function of void depth is seen. The results confirm that there is a peak in the secondary electron coefficient ratio and that the backscattering electron coefficient ratio decreases steadily with increasing void thickness.
Figure 19. Secondary and backscattering coefficient ratios for a specimen containing a cubic void at a depth of 200 Å. The calculations are for 9000 incident electrons.
Table 6. Ratios of secondary and backscattering electron coefficients for parallelepiped voids at depths of 500 Å, 700 Å, and 900 Å

<table>
<thead>
<tr>
<th>Void depth Å</th>
<th>Void thickness Å</th>
<th>Void length Å</th>
<th>Void width Å</th>
<th>δ void/δ solid</th>
<th>η void/η solid</th>
</tr>
</thead>
<tbody>
<tr>
<td>500</td>
<td>200</td>
<td>1000</td>
<td>1000</td>
<td>1.06</td>
<td>0.94</td>
</tr>
<tr>
<td>500</td>
<td>500</td>
<td>1000</td>
<td>1000</td>
<td>1.01</td>
<td>0.88</td>
</tr>
<tr>
<td>700</td>
<td>100</td>
<td>1200</td>
<td>1200</td>
<td>1.01</td>
<td>0.96</td>
</tr>
<tr>
<td>700</td>
<td>200</td>
<td>1200</td>
<td>1200</td>
<td>1.04</td>
<td>0.93</td>
</tr>
<tr>
<td>700</td>
<td>500</td>
<td>1200</td>
<td>1200</td>
<td>0.99</td>
<td>0.86</td>
</tr>
<tr>
<td>900</td>
<td>100</td>
<td>2000</td>
<td>2000</td>
<td>1.03</td>
<td>0.96</td>
</tr>
<tr>
<td>900</td>
<td>200</td>
<td>2000</td>
<td>2000</td>
<td>1.04</td>
<td>0.92</td>
</tr>
<tr>
<td>900</td>
<td>300</td>
<td>2000</td>
<td>2000</td>
<td>1.03</td>
<td>0.91</td>
</tr>
</tbody>
</table>

Several trends can be seen in these figures and tables. The backscattering coefficient ratio steadily decreases as the size of the void increases. This is due to the fact that as the size of the void increases the electron travels a longer distance inside the void and the new termination point of the recorded history is deeper inside the specimen. Therefore, the electron must pass through more material in order to escape the specimen and since the probability of electron absorption increases with increasing thickness of material the backscattering coefficient should decrease as the size of the void increases. The pattern of the secondary electron...
coefficient ratios is a peak in the ratio at a void thickness of 150 Å or 200 Å and a steady decrease of the ratio as the thickness of the void increases. This peak in the ratio is thought to be due to the interaction of two factors that help determine the secondary electron coefficient. The first is the probability that an electron that originally backscattered from the solid specimen will not come close enough to the surface to produce secondary electrons after passing through the void. Since this probability increases as the void thickness increases this will tend to decrease the secondary electron coefficient for a specimen containing a void. The second factor is the increase of the energy loss per unit path length because an increase in the size of the void increases the additional distance the electron must travel to reach the secondary production region. This factor will tend to increase the secondary electron coefficient for a specimen containing a void. The combination of these two factors leads to the peak in the secondary electron coefficient ratio curve. The ratio steadily decreases because the first factor begins to dominate in the determination of the number of secondary electrons produced as the void thickness is further increased.

To understand why these patterns re-occur it is necessary to understand the role of the geometric variables in determining the termination position of the recorded history which
in turn determine the coefficient ratios. The void cross-sectional area partially determines (a) the number of primary electrons that cross the top of the void on their path into the specimen, (b) the number of electrons that enter the bottom of the void, and (c) the distance the electron travels inside the void by setting the limits on the electron's travel in the X and Y direction.

The void thickness also helps determine the distance the electron travels inside the void by setting a limit in the Z direction of travel. The void thickness partially determines the number of electrons that enter the bottom and sides of the void. This is because the backscattered electron pattern becomes more diffuse as it approaches the surface and the deeper the bottom of the void the greater the probability than an electron will enter the bottom or sides of the void.

The void depth partially determines the number of electrons that enter the top of the void. The deeper the void, the greater the probability of an electron backscattering before reaching the void. For a void of given cross-sectional area, the deeper the void the greater the number of electrons that miss it. This is due to the spreading of the electron pattern as the electrons enter the specimen. In conjunction with the void thickness, the depth partially determines the number of electrons entering the bottom of the
Therefore, all geometric variables can enter into the determination of the backscattering and secondary electron coefficient ratios. However, for the cases considered in these calculations the major variable that determines the change in the backscattering and secondary coefficients is the void thickness. This accounts for the repetition of patterns at different depths.

Based on the results it is possible to predict changes in the coefficient ratios for larger voids. If the void thickness is increased further, at a given depth, the coefficient ratios will decrease as thickness increases. The coefficient ratios will approach 1.0 if the void depth is increased because the number of electron histories that backscatter before reaching the void will increase and the coefficient values will approach those of a solid specimen. If the cross-sectional area of the void is increased to the point where it measures about one square micron, the void will substantially cover the backscattered electron exit area of a copper specimen and the coefficient ratios will approach 1.0 because the electrons will travel nearly equal path lengths through the void when they are headed away from and towards the specimen surface.

Subsurface void contrast for specimen and SEM variables can be analyzed using the results of these calculations.
and the relationship between the scattering cross section and energy loss equation and these variables. The variables we are interested in studying are the chemical composition of the specimen (i.e., atomic number $Z$), the energy of the incident electrons, and the incident angle of the electron beam. In general the backscattering and secondary coefficients for a solid specimen increase with increasing atomic number, decrease with increasing incident electron energy, and increase as the angle of beam incidence decreases from 90 degrees.

The effects of subsurface voids on the backscattering and secondary coefficients for different atomic number specimens can be analyzed by determining the dependence of the probability of scattering and rate of energy loss on $Z$. The probability of scattering is proportional to $Z^2$ and the rate of energy loss is proportional to $Z$. Therefore, the probability of an electron being absorbed while traveling through a thin specimen is greater the higher the atomic number. The trends of the backscattering and secondary coefficient ratios are functions of the distance between the end point of the recorded history and the surface. This in turn was found to be a function of the void thickness in the calculations. Therefore, one would expect that the backscattering coefficient ratio for a given void would be less than that calculated for copper if the atomic number of the specimen was
greater than 29. Conversely, if the atomic number was less than 29 one would expect a ratio greater than that calculated for copper for a given void size. The changes in the secondary electron coefficient ratio for different atomic number specimens should be similar to the changes in the back-scattering electron coefficient ratio because the absorption of the backscattered electrons should decrease the secondary electron yield more than the increase in the energy loss per unit path length should increase the secondary electron production.

The case of different incident electron energies can be analyzed in the same way. The probability of scattering is proportional to $1/E^2$ and the rate of energy loss is proportional to $1/E$. Therefore, for a higher incident electron energy the trends observed for the 20 keV case should occur for thicker voids. For lower incident electron energies the trends should be observed for thinner voids.

The case of a change in the incident electron beam angle can be analyzed in the same way. For an incident beam angle of less than 90 degrees, the electron penetration is less than for the 90 degree beam incident case. Therefore, the probability of an electron backscattering at a depth less than the void depth is greater for an incident beam angle of less than 90 degrees than for an incident beam angle of 90 degrees. However, the electrons that do pass through the void
will be at a higher energy when they backscatter from the specimen because of the shorter distance they have to travel in order to reach the surface. Since the backscattered electrons have a higher energy, the probability of them being absorbed after passing through a void is less in the case of a tilted beam than in the case of the perpendicularly incident beam. Therefore, one would expect that the backscattering electron coefficient ratio for an angle of incidence less than 90 degrees would be closer to unity than for the 90 degree incidence case and the number of voids visible should be less and the contrast of the voids should be reduced in a micrograph taken with a tilted beam than one taken with a perpendicularly incident beam.

The secondary electron coefficient ratio for the tilted beam can be analyzed by considering the fact that the electrons that pass through the void and backscatter will be at a higher energy in the tilted beam case than in the perpendicular case. This means the probability of escape is greater and the energy loss per unit path length is less. Both of these factors will tend to make the secondary electron coefficient ratio closer to unity in the case of the tilted beam than in the case of the perpendicular beam. Therefore, one would expect less secondary electron subsurface void contrast in the tilted beam case than in the perpendicular beam case.
Examination of a Specimen Containing Voids Using the SEM

In order to confirm the results of these calculations, i.e. that subsurface voids do provide a significant contrast mechanism, a specimen containing voids was examined using the SEM. The examination was made not only to confirm the calculational results but also to observe the characteristics of subsurface voids. The specimen examined was a doped powder metallurgy tungsten light bulb filament. This specimen was chosen because it was easily obtained, nonradioactive, and contained a wide variety of void sizes. The specimen examined in this study was a tungsten filament from a 200 watt Westinghouse light bulb.

The introduction of small amounts of impurities into tungsten for the purpose of obtaining non-sag properties has been practiced for years. The introduction of \( K_2O \), \( SiO_2 \), and \( Al_2O_3 \) in the tungsten oxide prior to reduction by hydrogen to tungsten powder affects the recrystallization behavior of sheet and wire products manufactured from this powder. Moon, Stickler, and Wolfe (67) have studied the properties of sintered doped tungsten powder ingots. They found that 90% of the dopant material is volatilized and diffuses out of the material when the doped tungsten is annealed. They found that aluminum and silicon are reduced to low concentrations during heating to 2150 °C. While oxygen is reduced
to low levels only on heating to 2900 °C. The potassium content is reduced on heating to 2150 °C and 2900 °C but remains at a relatively high concentration after annealing at this higher temperature. It is believed that this high concentration can be accounted for by the fact that clusters of the K impurity atoms are trapped on the grain boundaries and attract vacancies from the surrounding lattice to form "embryo bubbles". Further impurities are attracted to the bubbles during annealing and the bubbles grow. At the annealing temperatures, the K impurity is volatilized and forms bubbles but when the wire is cooled the K condenses and a void is left in the tungsten metal.

The fact that the impurities formed cavities in the tungsten filaments was not definitely established until the early 1970's. When the tungsten filament is annealed it forms elongated crystals whose long axes are parallel to the working direction of the wire, which is the <110> crystal direction. The unannealed grains in the tungsten metal have a width of 0.5 μm while the annealed grains have a width as great as 20 μm. The effect of gas bubbles on the recrystallization of tungsten has been studied by many researchers but Koo (68) was the first to suggest and present evidence that the impurity formed bubbles and voids in the tungsten. Koo based this conclusion on the contrast observed in transmission electron micrographs. Das and Radcliffe (69) studied the
void formation as a function of annealing temperature. They found that the voids had been formed in rows, called stringers, which corresponded to the grain boundaries of the unannealed tungsten. At a temperature of 2200 °C the grains reached their full size. They found that the cavities were voids and that the average void diameter was 1500 Å. Their study was carried out using replicas and thinned specimens. Parrel, Schaffhauser, and Houston (70) reached the same conclusions in studying the effect of gas bubbles on the recrystallization of vaporized tungsten films. Moon and Koo (71) studied the mechanism and kinetics of bubble formation in doped tungsten. They explained the formation of the bubbles by studying replicas of the voids and thin films of doped tungsten ingots and sheets in the transmission electron microscope. They found that the voids reached their full size at temperatures above 2000 °C and an annealing time of 15 minutes. They observed sizes ranging from 150 Å to 5000 Å in diameter.

Based on these previous observations one would expect to find voids of an average size of 1500 Å in diameter after annealing a filament for more than 15 minutes. The specimen examined in this study was annealed in a vacuum at a temperature between 2000 and 3000 °C for one hour by burning the light bulb for one hour.

To show that subsurface voids do provide a contrast mech-
anism it is necessary to identify these subsurface voids in the Scanning Electron Micrographs. This identification was done by removing the material on top of the void and examining the open void on the surface of the specimen. The technique used was to make a micrograph of the specimen with the voids and then etch away a small amount of the material using an ion mill. The same area of the specimen was examined again and a micrograph made. The specimen was again etched and the process was continued until the subsurface void was a pit on the specimen surface. The etching was done on an ion mill with 0.4 milliamps current at 5 kilovolts using argon ions and typically 200 Å of the material was removed per 0.1 hour of etching.

Figure 20 shows the specimen mounted in the ion mill sample holder. The specimen was mounted in this holder throughout this series of observations and etches to insure that the observation geometry and the etching geometry remained constant during this study. The micrographs were made using a Cambridge Stereoscan SEM equipped with a LaB₆ electron source. The SEM was operated at 20 keV with the specimen normal to the electron beam unless otherwise noted in the description of the micrographs.

The sequence of micrographs that demonstrates subsurface void contrast is shown in Figures 21 through 29. The micrographs concentrate on two subsurface voids that are barely
Figure 20. Tungsten filament mounted in the ion mill sample holder

Figure 21. Micrograph of the unetched filament showing three voids. The area in the middle of the triangle formed by the three voids contains two deep subsurface voids

Figure 22. Micrograph of the tungsten filament after 0.1 of an hour of etching. The two subsurface voids are in the center micrograph and appear as two faint dark areas

Figure 23. Micrograph of the tungsten filament after 0.2 of an hour of etching. The two subsurface voids are in the center of the micrograph. The contrast of the voids is increased as compared to the contrast in the un-etched specimen
Figure 24. Micrograph of the tungsten filament after 0.3 of an hour of etching. The subsurface voids are in the center of the micrograph. Void A has a circular form and the contrast of both voids is increased because material has been removed from on top of the voids.

Figure 25. Micrograph of the specimen area analyzed for subsurface voids after 0.5 of an hour of etching. The subsurface voids are in the center of the micrograph. Void A is now on the surface but void B is below the surface.

Figure 26. Micrograph of the specimen area analyzed for subsurface voids after 0.7 of an hour of etching. The voids are in the center of the micrograph and both are on the surface.

Figure 27. Micrograph of the specimen area analyzed for subsurface voids after 0.9 of an hour of etching. The voids are in the center of the micrograph. The walls of both voids are visible and part of the bottom of one of the voids is visible.
Figure 28. Micrograph of the specimen area analyzed for subsurface voids after 1.2 hours of etching. The voids are seen in the center of the micrograph. The bottoms of both voids are visible. Note that the outline of the voids is not a true circle indicating a possible coalescence of smaller voids.

Figure 29. Micrograph of the specimen area analyzed for subsurface voids after 1.5 hours of etching. The remnants of the subsurface voids are visible in the center of the micrograph. The bottoms of the voids are slightly below the surface.

Figure 30. Micrograph of an area of the specimen taken with the electron beam perpendicular to the specimen surface. Many subsurface voids are visible.

Figure 31. Micrograph of the area of the specimen shown in Figure 30 taken with the specimen tilted at an angle of 40 degrees with respect to the incident beam. The contrast of the subsurface voids is greatly reduced in comparison with the voids shown in Figure 30.
visible in the first micrograph and gradually are brought
to the surface of the specimen by etching away surface
material. The etching is continued until the bottoms of
these voids are clearly visible in the micrograph.

Figure 21 is a micrograph of an area of the unetched
specimen. There are three definite voids in the micrograph
which form a triangle in the lower center of the micrograph.
Inside this triangle two slightly darker areas can be seen
and in later micrographs it will be shown that these darker
areas correspond to subsurface voids. Figure 22 shows the
area of the specimen after 0.1 hour of etching. The area
that contains the two subsurface voids is now in the center
of the micrograph. The contrast due to the two subsurface
voids is slightly increased but it is still substantially
lower than that observed for the other voids visible in the
micrograph. Figure 23 shows the same general area of the
specimen after 0.2 hour of etching. The two subsurface voids
are visible in the center of the micrograph. These sub-
surface voids are referred to as voids A and B in the rest of
the discussion. The contrast of the two voids is now great
enough that void A is taking on a circular shape. Figure 24
shows the area of the specimen after 0.3 hour of etching.
About 600 Å of surface material has been removed at this
point. The two subsurface voids are in the center of the
micrograph. The contrast is sufficient so that void A has a definite circular shape but the shape of void B is still indeterminate. Note that a smaller void has appeared to the left and slightly below void B.

The next micrograph, Figure 25, shows the area of the specimen after 0.5 hour of etching. The two voids that we are interested in are near the center of the micrograph. Both voids now appear as distinct dark circles. Void A is thought to have had all the material on the top of the void removed by etching so that the void is now an open pit on the surface of the specimen. This is believed to be the case because of the light ring around the void. This ring is formed because of the increased secondary electron emission from the edge of the pit. Void B still appears to be below the surface.

Figure 26 shows the area of the specimen after 0.7 hour of etching. The center of the micrograph contains the two voids whose contrast we have been observing as a function of the material removed. Both voids are now pits on the surface of the specimen, as evidenced by the light ring around both of the voids. Also the wall of void A is visible in the micrograph. The specimen was next etched for an additional 0.2 hour so that in Figure 27 the specimen has been etched for a total of 0.9 hour. The two voids are in the center of the micrograph. The wall and part of the bottom of void A is visible and the wall of void B is visible. Note that the
voids do not form perfect circles on the surface of the specimen as was observed in Figure 26 but have definite features on the sides of the pits.

Figure 28 shows the area of specimen after 1.2 hours of etching. The two voids are visible in the center of the micrograph. The bottom and sides of both voids are visible. The outline of void B is irregular as compared to the smooth circular form visible in Figure 26. These features of void B were probably covered by some of the material in Figure 26 so they did not significantly affect the signal that formed the micrograph. Figure 29 shows the area of the specimen after 1.5 hours of etching. The subsurface voids that have been brought to the surface are visible in the center of the micrograph. The bottoms of both voids are seen in the micrographs. The bottoms of both voids are near the specimen surface due to the etching of the specimen. This series of micrographs shows that subsurface voids do provide a significant contrast mechanism that makes the subsurface voids visible in the micrographs.

The analysis of these micrographs indicates that the large voids are built from a coalescence of smaller voids. In Figure 27 a small void is visible in the bottom of a pit near the center of the micrograph below void B. This small void is thought to be a subsurface void because of the lack of
the light ring around the void. Also a small void is visible in the bottom of void A in Figure 29. The outline of void B in Figure 28 is suggestive of several smaller voids coming together to form the larger void.

One of the results of the theoretical study was that the number and contrast of subsurface voids visible in a micrograph made with the incident electron beam at an angle of less than 90 degrees should be less than for voids visible in a micrograph made with an electron beam angle of 90 degrees. This is because of the shallower penetration of the electron beam for the lower incident angle. This result was tested using the tungsten specimen. Figure 30 shows an area of the specimen after 1.5 hours of etching that contains a wide variety of voids. The largest void measures 3800 Å in diameter while the smallest void measures 400 Å in diameter. Figure 31 shows the same area of the specimen as Figure 20 but with the specimen tilted at an angle of 40 degrees with respect to the incident beam. The contrast of many of the voids is greatly reduced and some of the subsurface voids visible in Figure 30 are not visible in Figure 31. The fact that some of the surface features seen in Figure 31 are not seen in Figure 30 is because the tilt of the specimen gives a distorted field of view, and a slightly different area is seen in Figure 31 than in Figure 30. These two micrographs illustrate that subsurface void contrast is reduced by
tilting the specimen.

**Monte Carlo Method Applied to Multiple Element Systems**

Because the present Monte Carlo programs are only capable of handling specimen regions composed of a single element and because many materials in a reactor, particularly ceramic fuels, are composed of several elements, it is desirable to have a Monte Carlo algorithm that can be used for alloys and compounds. Using this type of simulation one could carry out calculations for cavities in ceramic nuclear fuels. Previously, multiple element systems have been handled by Nishigori et al. (31) using Lewis' multiple scattering theory and by Shimizu and Everhart (37) using single scattering theory. The best method to use should be single scattering theory because of its ability to simulate collisions with atoms of widely varying atomic number without having to combine the effects of many atoms of different atomic number in the simulation of one multiple scattering step. The technique used in this study is a modified single scattering theory for multiple element systems similar to the theory developed by Shimizu and Everhart (37). The derivation of the equations, the algorithm, and the computer program are given in Appendix B.

The multiple element system chosen to test this program
was a copper-gold alloy because of available experimental data. The program was used to compute the backscattering coefficient for various compositions of the alloy. In the program it was assumed that \( \rho = \sum \rho_j C_j \), where \( \rho \) is the alloy density, \( C_j \) is the weight fraction of the \( j \)th element, and \( \rho_j \) is the density of the element. The calculations were performed for 1000 incident electrons. The results are shown in Table 7 along with the experimental values of Bishop (72).

<table>
<thead>
<tr>
<th>Weight fraction of copper (%)</th>
<th>Weight fraction of gold (%)</th>
<th>Incident energy (keV)</th>
<th>Experimental coefficient</th>
<th>Calculated coefficient</th>
</tr>
</thead>
<tbody>
<tr>
<td>80</td>
<td>20</td>
<td>5</td>
<td>0.38</td>
<td>0.39</td>
</tr>
<tr>
<td>60</td>
<td>40</td>
<td>5</td>
<td>0.43</td>
<td>0.44</td>
</tr>
<tr>
<td>40</td>
<td>60</td>
<td>5</td>
<td>0.45</td>
<td>0.51</td>
</tr>
<tr>
<td>80</td>
<td>20</td>
<td>10</td>
<td>0.39</td>
<td>0.41</td>
</tr>
</tbody>
</table>

It is felt that the error in the calculations is about 3%. This is based on the observations of Kyser and Murata (73) that the error in the backscattering electron coefficient for single scattering Monte Carlo calculations is approximately \( \sqrt{n}/n \), where \( n \) is the number of incident electrons. Except in the case of the 40-60 alloy the calcu-
lated values are within this assumed calculational error of
the experimental values. The reason for this discrepancy is
not known but it is possible that the number of incident
electrons is too small.

Secondary electron calculations were not done for several
reasons. First, no experimental data could be found for this
alloy. Second, there are two possible ways of calculating
the secondary yield of an alloy. One could use a single value
of $\lambda_s$ throughout the entire electron history to calculate the
electron's secondary electron production. $\lambda_s$ for the alloy
is given by

$$\frac{1}{\lambda_s} = \sum_j \frac{1}{\lambda_{s_j}},$$

where $\lambda_{s_j}$ is the mean free path of secondary electrons of
each element. A second method that could be used is to
record which elemental atom the incident electron collides
with at the beginning of each step in the history and use
the mean free path of the secondary electron for this element
in the calculation of the secondary electron production of
this step in the history. Finally, one would have to choose
a value of $\lambda_s$ for gold since Seiler (59) gives two possible
values of $\lambda_s$ for gold and one would have to do calculations
on a gold specimen in order to choose a value of $\lambda_s$.

This program can be used for compounds such as uranium
dioxide. It is simply a matter of inserting the correct density, weight fractions, atomic weight, and atomic number into the program to calculate electron histories in this ceramic material. However, to calculate the secondary electron production would require knowledge of the mean free path of the secondary electrons in \( \text{UO}_2 \) because \( \text{UO}_2 \) is a nonconductor at room temperature and has a unique \( \lambda_s \). The program could be used for a mixed oxide fuel, such as \( \text{PuO}_2-\text{UO}_2 \), by computing an average density for the material and knowing the weight fractions of each element. Again, however, one would have to know \( \lambda_s \) for the compound in order to calculate the secondary production for the compound.

The effect of bubbles in ceramic nuclear fuels on the backscattering signal could be calculated using the scheme outlined for the single element material void analysis but using the Monte Carlo calculations for multiple element systems. The effect on the secondary electron production could be calculated if the value of \( \lambda_s \) is known for the compound.
CONCLUSIONS

This study was undertaken to better interpret Scanning Electron Micrographs of cavities in materials. Because of the features of the SEM, high magnification and high depth of field, study of cavities in reactor materials is practical and there should be increased use of the SEM for this purpose. In order to interpret these high magnification micrographs it is necessary to understand the role of subsurface cavities in signal formation in the SEM. This study has analyzed the role of subsurface voids using both theoretical and experimental techniques.

A theoretical analysis used a combined single and multiple scattering theory Monte Carlo method computer algorithm. This algorithm extends the previous use of these theories in the simulation of the interactions between the electron and the specimen by using the accuracy of single scattering theory only where it is needed and using the speed of multiple scattering theory to complete the rest of the electron history. The accuracy of single scattering theory is retained in the region of secondary electron production and in the region where voids are considered. The rest of the simulation uses multiple scattering theory.

Because of conflicting reports in the literature it was necessary to test the single scattering algorithm to determine
which expression for the screening angle should be used in the calculations. It was found that the expression derived by Nigam et al. gave results closest to published experimental findings. An empirical expression from Cosslett and Thomas (55) was used to determine the number of elastic scattering collisions to be simulated by one multiple scattering theory step. The value of $p_e = 22.6$ is within the experimental range of $p_e = 25 \pm 5$, as determined by Cosslett and Thomas. This was calculated from a comparison of single and multiple scattering theory calculations for electrons transmitted through thin specimens. Since all the secondary electron production results are expressed as ratios it is only necessary to know the mean free path of the secondary electrons in the element in order to calculate the secondary electron coefficient ratios. Based on a comparison with previous theoretical calculations and experimental results it was determined that the mean free path of the secondary electrons to be used in the calculations was 20 Å.

The combined single and multiple scattering theory algorithm computes backscattering and secondary electron coefficients that are in agreement with experimental results and single scattering theory Monte Carlo calculations for a copper specimen with 20 keV incident electrons. The backscattered electron histories produced by the combined single and multiple scattering theory program were used to
calculate the backscattering and secondary electron coefficients for specimens containing parallelepiped voids. By ratioing these values with the coefficients for the solid specimen the theoretical contrast ratios were calculated. It was found that both the backscattering and secondary electron coefficient ratios were a function of the void size but they were essentially independent of void depth for those depths considered. It was found that the cross-sectional area of the voids was not strongly related to the coefficient ratios and that the coefficient ratios were essentially a function of the void thickness.

The backscattering electron coefficient ratio decreased in nearly a linear fashion with increasing void thickness. This is because the thickness of the material that the electron must travel through in order to reach the surface increases with increasing void thickness. This corresponds to Cosslett and Thomas' (55) finding that the fraction of incident electrons transmitted through a thin copper specimen decreases linearly with increasing specimen thickness.

The secondary electron coefficient ratio reached a peak for a void thickness of 150 Å to 200 Å then decreased as the void thickness increased. The peak in the secondary electron coefficient ratio may be a function of the value chosen for the mean free path of the secondary electron.
This peak may occur because the secondary electron production region extends to a depth of 100 Å. In the calculations it was found that the void thickness was the major geometric variable. Consider a void with a thickness of 100 Å. The greatest depth at which the recorded electron history can now be terminated is 100 Å below the surface and all the electron histories that are continued using the single scattering theory Monte Carlo calculations must enter the secondary electron production region. Therefore, one would expect a secondary electron coefficient ratio greater than 1.0 for voids of 100 Å thickness. Since the probability of the backscattered electron spectrum passing through the 100 Å thickness of material is quite high it is possible that the secondary electron coefficient ratio could peak for the 150 Å to 200 Å thick voids. If a smaller value of \( \lambda_s \) were used this might not be the case.

The range of the calculated backscattering electron coefficient ratios was from 0.97 for a (50 Å)\(^3\) void at a depth of 50 Å to 0.65 for a (1000 Å)\(^3\) void at a depth of 100 Å. The secondary electron coefficient ratios ranged from a high of 1.08 for a (200 Å)\(^3\) void at a depth of 100 Å to a low of 0.93 for a (1000 Å)\(^3\) void at a depth of 100 Å. These values are the range of the calculated secondary and backscattering electron contrast for subsurface voids that might be visible in micrographs of a copper specimen using
20 keV incident electrons. According to Rose (74), the minimum change in contrast that is visible to the human eye is 0.05. This means that the contrast ratios must be greater than 1.05 or less than 0.95 for the subsurface void to be visible. Therefore, voids with thicknesses greater than or equal to 100 Å should be visible in the micrographs using the backscattered electron signal. The 150 Å or 200 Å thick voids may be barely visible as light areas in micrographs using the secondary electron signal. Voids of 1000 Å or greater thickness should be visible as dark areas in secondary electron micrographs but voids with thickness greater than about 150 Å to 200 Å and less than about 1000 Å will be invisible using this criteria. However, by using differential amplification in the signal processing (black level processing on the Cambridge SEM and gamma processing on the JEOL SEM) it is possible to see much lower contrast variations. The visible contrast variation may be as low as one percent using this signal processing. Using this criteria all the voids would be visible using the backscattering electron signal and the only voids that would not be visible using the secondary electron signal would be 600 Å to 700 Å thick voids. Therefore, the calculations predicted that subsurface voids should be a significant source of contrast in the SEM and that the contrast is proportional to the size of the void.
Calculated values of the backscattering and secondary electron coefficient ratios for a \((600 \, \text{Å})^3\) void at a depth of 100 Å obtained using a program that considered the possibility of electrons passing through the side of the void and another program that neglected the possibility of an electron entering through the side of the void were compared and were found to be within the calculated error of each other. Based on this analysis the calculational approximation can be made that the electrons only enter the top and bottom of the void for voids thinner than 600 Å. For thicker voids the passage of electrons through the sides of the voids should be considered.

Based on the calculations and an analysis of the cross sections as a function of material, electron energy, and beam angle the following conclusions can be drawn. The void contrast should increase as the atomic number of the material increases but the voids must be at a shallower depth to interact with the electrons. The void contrast should increase as the electron beam energy decreases but the voids must be closer to the surface to interact with the electrons. The void contrast should approach unity as the angle of beam incidence decreases.

These calculations can be used to predict possible sub-surface void contrast in a ceramic nuclear fuel such as uranium dioxide. Since \(\text{UO}_2\) has an average atomic number of
36 and 0.0669 atoms per cubic angstrom one would expect it to have electron scattering and absorption properties similar to those of yttrium or zirconium, which have similar Z and number of atoms per unit volume. Bubbles in the ceramic nuclear fuel will contain fission gases. Since the number of atoms per unit volume for gases is 2 to 3 orders of magnitude less than that of a solid, the probability of the electron scattering while passing through the bubble is small compared to its scattering probability in the solid fuel. Therefore, the contrast due to subsurface fission gas bubbles in UO$_2$ in the SEM should be similar to that of voids in yttrium or zirconium. Therefore, subsurface bubbles should be visible in micrographs of ceramic nuclear fuel and the relationship between the contrast and the size of the bubble should be similar to that observed for voids in intermediate atomic number metals.

These calculations have been performed for an idealized geometry; the voids were parallelepipeds with one face parallel to the surface. The voids observed in actual specimens range from spheres to multisided three dimensional figures and the faces may be at various angles with respect to the surface. The result of modeling these actual voids with the idealized geometry is to enhance the effect of the subsurface voids. This is because the geometry used in the calculations intercepts more of the electrons and the electrons travel further inside the void than they would in actual voids. Therefore,
contrast ratios calculated for the rectangular parallelepiped voids are greater than those that would occur for spherical or multisided voids.

Actual voids in materials do not occur in as idealized a situation as considered in the calculations. It is necessary to consider the effect of other phenomenon that occur in specimens containing voids on the contrast of subsurface voids. Often specimens containing voids have segregation or precipitation of impurity or solute atoms at the void-matrix interface. This phenomenon would increase the visibility of subsurface voids by providing a source of increased scattering and contrast at the boundary of the void. This would tend to increase the contrast between the void and the surrounding material. Also, overlapping voids are often observed in specimens. Since the backscattering and secondary electron coefficients depend on the distance the incident electrons travel inside the void, the effect of overlapping voids is to make the contrast of the overlapping voids the same as the contrast for a large void of size equivalent to the combined size of the overlapping voids. Therefore, the contrast of two overlapping voids would be greater than the contrast due to a single void. Also, overlapping subsurface voids would be indistinguishable from a single subsurface void in SEM micrographs. This was demonstrated in the voids shown in the SEM micrographs of the
tungsten specimen. Finally, the SEM has a beam of finite diameter while the calculations considered a beam incident at one point on the specimen surface. The effect of using a finite beam in the calculations would be to increase the spread of the electron pattern in the specimen. Therefore, more electrons would backscatter without passing through the void in the case of a finite diameter beam than in the case of the beam incident at a point on the surface. Therefore, the backscattering and secondary electron coefficient ratios would be closer to unity for the finite diameter beam than for the beam incident at a point on the surface of the specimen.

The micrographs of the voids in the doped tungsten filament show that the subsurface voids do provide a significant contrast mechanism for specimens containing voids. The subsurface void contrast increases with void size which corresponds to the results of the theoretical calculations. The calculations predicted that the void contrast should be less than 1.0 for void sizes of at least (1000 Å)³ in a copper specimen. The fact that all voids visible in the tungsten specimen appear as dark areas confirms the prediction that the contrast should decrease sharply as the void thickness increases for higher atomic number materials. The fact that the number of subsurface voids resolved in the micrograph of the tilted specimen is less than the number resolved in a perpendicular beam micrograph confirms the prediction.
that the use of a lower angle will reduce the subsurface void contrast. Finally, the subsurface void measures approximately the same size as the void when it is on the surface of the specimen. Therefore, one can conclude that subsurface voids provide a significant contrast mechanism which results in a signal that is characteristic of the size of the void.

The Monte Carlo method can be used for electron history simulations in multiple element systems. The algorithm using the single scattering theory gives backscattering coefficients for a copper-gold alloy that are within the calculated error of the experimental values. This method can be used for any alloy or compound and could be used as the basis of a subsurface void analysis program for multiple element systems. The secondary electron production programs for multiple element systems require more development before they can be used for alloys or compounds.

Therefore, the SEM is an excellent tool to examine cavities in specimens. With the field emission source the SEM provides a high magnification and large depth of field instrument that can be used to examine a large range of bulk specimens. The subsurface voids must be considered in the interpretation of micrographs of specimens containing voids. However, rather than being a problem, the subsurface voids provide additional information about the
specimen. The fact that subsurface voids can be seen in micrographs means that the micrograph is representative of a small volume of the material rather than just the surface of the material. By knowing the mean penetration depth of backscattering electrons one could approximate the volume of material analyzed in the micrograph. Using this volume and the calculated volume of the voids a direct measure of the percentage of the material taken up by the voids is available from the SEM micrographs. These results apply to voids or bubbles in ceramic or metallic reactor materials. The mean penetration depth of backscattering electrons ranges from about one micron in low atomic number materials to a few hundred angstroms in high atomic number materials.

If subsurface cavity contrast is a problem, the number of cavities that are visible can be reduced by two methods. The incident electron beam energy can be lowered so that the penetration depth is less or the angle of beam incidence can be decreased from 90 degrees so that the penetration depth is again reduced. Either of these methods reduces the number of subsurface voids with which the electrons can interact.

The Monte Carlo method simulation can be applied to both single and multiple element specimens. Therefore, simulations could be carried out for ceramic nuclear fuels or other compounds. Combining this capability with the capability of using a virtually infinite number of geometries,
where various sections of the specimen can be composed of different materials, the Monte Carlo method can be used to simulate interactions in specimens which can be observed in the SEM. The Monte Carlo method can provide basic information about the electron interactions with the specimen which is required for an exact interpretation of SEM micrographs.
SUGGESTIONS FOR FURTHER RESEARCH

The power of the Monte Carlo method is the broad range of interactions between electrons and the specimen that can be analyzed. The void analysis technique could be repeated for different element specimens, electron energies, and angles of beam incidence to determine the exact effect of changing these variables. Calculations could also be done using other void shapes and orientations to see the effect of more realistic void geometries on the contrast. Another possibility would be to use a finite width beam in the calculation to see the effect of using a more realistic beam on the contrast due to subsurface voids.

An analysis of the change in the low energy loss back-scattered electrons could be performed to determine the effect of subsurface voids on this signal. It is expected that the most probable energy of the backscattered electron distribution from a specimen containing a void will be less than that for a solid specimen.

The subsurface cavity analysis can be extended to ceramic nuclear fuel using the multiple element Monte Carlo method described in Appendix B. Some consideration should be given to using Lewis' multiple scattering theory for multiple element systems in the calculations. These programs could determine the backscattering coefficient ratios for any
compound or alloy. Secondary electron coefficient ratios could be determined for alloys using the secondary electron mean free paths of each element but to use the secondary production programs for compounds requires prior knowledge of the secondary electron mean free path for the compound.

Several other specimen configurations could be simulated to determine the theoretical effects of the electron interactions with the specimen in the SEM. Calculations could be performed to analyze the theoretical resolution of the SEM for different features on the surface of the specimen. This could be done by using two identical features on the surface of the specimen with the electron beam incident on one feature in one calculation and in between the two features in a second calculation. The distance between the features can be changed and the changes in the backscattering and secondary coefficients analyzed. The theoretical limit of resolution could be determined by noting when the difference between the coefficient for the beam incident on the feature and the coefficient for the beam incident between the features is below a certain level. The Monte Carlo method could also be used to analyze the effect of the coating thickness on the secondary and backscattering coefficients to determine the relationship between signal strength and coating thickness.

Monte Carlo method simulations could also be done for the interaction between the electron beam and the specimen
in the Scanning Transmission Electron Microscope (STEM). However, more precise theories of electron scattering and electron energy loss would probably have to be used because of the higher electron energies used in the STEM and because of the small number of collisions the electron suffers while going through the specimen. This latter situation requires more precise modeling of each collision than given by the Rutherford cross section. Berger (21) gives some suggestions on possible cross sections to use. However, before these analyses are made certain theoretical problems should be resolved in order to better use the Monte Carlo method in the simulation of the interaction between the electron and the specimen.

More work needs to be done in the area of secondary electron production. Murata (38) has suggested that the use of the Bethe continuous energy loss equation tends to overestimate the contribution of $\delta_p$ to the total secondary electron coefficient. Comparisons of the calculated secondary electron production parameters with experimental measurements of known precision using the Bethe energy loss equation and more advanced theories of electron energy loss such as the theories outlined by Spencer and Fano (75) or Rohrlich and Carlson (76), are required to determine which energy loss theory should be used in the calculations. This should definitely be done before any calculations are done where changes in $\delta_p$ may significantly affect the results. The Bethe theory
is adequate for cases where changes in $\delta_n$ are significant because the Bethe theory agrees with the more advanced theories for the backscattered electron energies for incident beam energies of less than 30 keV.

More experimental information is needed for secondary electron production in alloys and compounds. Data is needed for the value of $\delta$ for compounds and alloys in order to check the calculations. Values of $\lambda_s$ for compounds are needed to calculate $\delta$ for compounds.

The SEM could be used to analyze a specimen containing subsurface voids and a comparison made with the results of an analysis using replicas of the surface. This would provide a comparison between the topographical information of a specimen given in a micrograph of the replica and the combination of surface and subsurface information given in a SEM micrograph. However, it is uncertain that any more information could be gained about the specimen surface using the replica technique than from the tilted beam SEM micrographs. Plastic replicas have a practical resolution limit on the order of a few hundred angstroms (11) so that information about small voids may be lost. Also, it might be difficult to strip the replica from the surface because of the plastic getting into vase shaped voids on the specimens surface and the replica might tear when an attempt is made to remove it. It would not be possible to use evaporation
replicas using carbon or a metal because, according to Murr (77), these replicas cannot be stripped from the specimen surface for observation.

Measurements of the volume fraction taken up by the voids could be made by examining the voids in the SEM micrographs and determining the maximum depth of electron penetration using the Monte Carlo method, which can be used to determine the volume of material analyzed in the micrographs. The fact that the SEM can be used to successfully analyze voids in a specimen should encourage the use of the SEM in the analysis of radiation damaged materials.

The Monte Carlo method can be used for any charged particle transport problem. The equations can be simply modified to take into account relativistic energies. Other modifications might have to include more complex interactions such as X-ray production and knock on electrons in the case of higher incident energies. These modifications are not too difficult to make. Therefore, the method provides a powerful tool for analyzing charged particle transport in complex geometries.
LITERATURE CITED


ACKNOWLEDGMENTS

The author wishes to express his appreciation to Drs. Raymond T. Greer, Richard A. Danofsky, John D. Verhoeven, Laurent Hodges, and Alfred F. Rohach who formed his graduate committee. Special thanks are due to Dr. Raymond T. Greer for his advice and encouragement given the author during this investigation. Thanks are also due Dr. Michael R. Ringham for his assistance during the initial stages of this study.

The author wishes to express his gratitude to Dr. John D. Verhoeven and the Metallurgy Division of Ames Laboratory for the use of the Cambridge SEM. Without it the experimental study could not have been completed.

The author wishes to thank the National Science Foundation for the traineeship under which this work was accomplished and which has supported him during his graduate studies. Thanks are also due the Iowa State University Engineering Research Institute and the Department of Chemical and Nuclear Engineering for their support of this investigation.

The author would like to express his gratitude for the support given him by Dr. and Mrs. B. F. Jackson. Finally, the author wishes to thank his wife, Juli, for her encouragement, patience, and understanding during this investigation.
APPENDIX A - PROGRAMS USED IN THE ANALYSIS OF SUBSURFACE VOID CONTRAST

Monte Carlo Method Programs

These programs compute completed electron histories for an electron beam incident to an infinitely thick specimen. The user must provide the initial energy of the electron (in eV), the angle of incidence of the electron beam, and the geometry and composition of the specimen. The total model is composed of three programs (1) the single scattering Monte Carlo program, (2) the multiple scattering Monte Carlo data program, and (3) the combined multiple and single scattering theory Monte Carlo program.

The execution of the program package proceeds as follows:

(1) Select the region in which the single scattering theory Monte Carlo calculations are to be performed. This will either be an area which contains boundaries or an area where secondary electrons can escape from the specimen.

(2) Select the incident electron energy (in eV), angle of beam incidence, the constant for the screening angle (it is recommended that the Nigam et al. (48) value of 5.449 be used in the calculations), the random number seeds, and material data (atomic number, atomic mass, density, and ionization constant).

(3) Insert these values into the single scattering
theory Monte Carlo program which outputs the energies of the electrons at the bottom of the region in which single scattering is to be used.

(4) Based on an examination of this electron energy distribution at the bottom boundary of the single scattering region choose the initial energy at which multiple scattering theory is to be used. The selection of this energy is discussed in the Results and Discussion section. Equations 32, 54 and 55 are used to determine the number of multiple scattering steps required to reduce the electron energy to the minimum electron energy that is used in the calculations.

(5) Insert the initial multiple scattering energy, material parameters, and number of multiple scattering steps into the multiple scattering data program. The step length, energy, and rate of energy loss for each multiple scattering step is recorded on magnetic tape. The integral cross section for the polar scattering angle is calculated and the values of the angles, which correspond to 91 equally distributed values of the cross section between zero and one, are recorded on magnetic tape. These angular values are recorded for each step.

(6) Select input parameters for execution of combined theory program:

(a) Select and input the electron beam energy (in eV), the angle of beam incidence, the constant for the screening
angle, the number of histories desired, the size of the random number vector (this will depend on the core size of the computer), the random number seeds, and the material data.

(b) Select the desired geometry and translate the geometry into the necessary IF statements required by the subroutine FATE. The basic technique is to assign region numbers to each homogeneous region within the specimen and set up boundaries between the regions. The IF statements are designed to check if an electron moves from one region to another. Boundaries are established to separate physically different regions or are inserted to allow the program to record the electron data at certain points within the specimen. If boundaries separate physically different regions the correct material data must be used in the program for each region and all material data must be initially put into the program.

(7) Execute the combined theory Monte Carlo program. The program reads a set of multiple scattering data. This data is the step lengths, energies, rates of energy loss, and the values of the polar scattering angle. The program starts the histories using the single scattering model in the region where single scattering is specified. Once the program is out of this region the single scattering model is continued until the electron reaches a multiple scattering energy. The program then follows the trajectory using the multiple
scattering model until (1) the electron reaches a depth greater than the remaining multiple scattering path lengths, (b) the number of multiple scattering steps is exhausted, or (c) the electron returns to the region where single scattering is required. In this last case the electron trajectory is continued using the single scattering model until the electron is backscattered or its energy is reduced to 2% of the incident energy. In this program the portion of the backscattered electron histories that are in the single scattering region are recorded on magnetic tape. The logic diagrams and program listings of the single scattering theory Monte Carlo program, the multiple scattering theory data program, and the combined single and multiple scattering theory Monte Carlo program appear on the following pages.

All the programs given in this appendix have the data inserted to produce electron histories in a copper specimen using 20 keV electrons perpendicularly incident to the specimen surface. If a user desires to run the programs for another case he must insert the proper data using the assignment statements in the programs.
Single scattering Monte Carlo program

Start

Enter random number seeds

Initialize constants for the calculations

Enter incident electron energy and position

Enter boundary positions

Calculate distance between boundaries

Enter number of electron histories desired

Enter material dependent parameters for each material. Enter atomic number, atomic mass, material density, and the value of the ionization constant.

Form random number vectors

Have all histories been calculated?

Yes

Stop

No

Initialize electron parameters

1

Figure A1. Logic diagram of the single scattering theory Monte Carlo program
1. Initialize material and region dependent constants
2. Calculate the value of the screening angle
3. Calculate the macroscopic cross section or $1/\lambda$
4. Calculate the energy loss per unit path length
5. Calculate the path length the electron travels
6. Calculate the corresponding Z coordinate

Does the electron cross a boundary?

- Yes
  - Calculate the new electron coordinates, macroscopic cross section, energy loss per unit path length, and energy
  - Record the electron parameters if electron is in secondary electron production region
  - Calculate the azimuthal, $\alpha$, and polar, $\beta$, scattering angles with respect to the direction of the electron travel in the previous step
  - Calculate the azimuthal, $\phi$, and polar, $\theta$, scattering angles with respect to the incident electron beam direction

- No
  - Calculate the new electron coordinates, macroscopic cross section, energy loss per unit path length, and energy

Figure A1 (Continued)
Is the number of collisions greater than 400?

No

Is the electron energy less than 4 keV?

No

Calculate the electron parameters at the boundary and record these parameters.

Does the electron cross the upper or lower specimen boundary?

No

Set material parameters for the next region

Yes

Figure A1 (Continued)
Calculate the macroscopic cross section, energy loss per unit path length, and path length the electron must travel in this new region to complete the previously calculated path length.

Calculate the corresponding Z coordinate in the new region.
SINGLE SCATTERING MONTE CARLO PROGRAM

THIS PROGRAM USES THE SINGLE SCATTERING THEORY FOR MONTE CARLO CALCULATIONS OF ELECTRON BEAM INTERACTIONS WITH A SINGLE ELEMENT PER SPECIMEN REGION. I.E. NOT FOR ALLOYS.

THIS PROGRAM IS DESIGNED FOR THIN SPECIMEN PROBLEMS. THE SPECIMEN THICKNESS SHOULD NOT EXCEED 2 OR 3 MULTIPLE SCATTERING THICKNESSES.

FOR NONRELATIVISTIC INCIDENT ELECTRON ENERGIES. IF THICKER SAMPLES ARE CONSIDERED THEN TERMINATION BECAUSE OF NUMBER OF COLLISIONS AND ENERGY OF ELECTRON SHOULD BE CHANGED.

REAL*8 S1, S2, S3
REAL*4 I, IAL, IC ISI, IAU
DIMENSION RHC(7), RPL(3000), RAT(3000), RAP(3000), NPW(163)
COMMON NREG, Z0, ZB4, ZB3, ZB2, ZB1, ZB0, NAB, ZI, XI, S, SIN, COS, YI, SINF,
1E, DES, SI, CS, SIP, SIG, CD, CE, X, NTYPE, NOUT, EA, CECU, CXCUC, CSCU, ICU, SIGS,
1COST, CX, ZP1, ZP2, ZP3, ZP4, ZP5, ZP6, ZP7, ZP8, ZP9, ZP10, ZP11, ZP12, ZP13, ZP14, NP, NW1
COMMON ZB11, ZB12, ZB13, ZB14
NW1 = 9
NW2 = READ / WRITE UNIT FOR WRITING PARAMETERS FOR ALL BOUNDARIES
NW2 = 10
CROSSED
NW2 = READ / WRITE UNIT FOR WRITING PARAMETERS AT CROSSING OF LOWER BOUNDARY
MRAN = 3000
MRAN = SIZE OF RANDOM NUMBER VECTOR
NRPR = 1
NRPR = COUNTER FOR RECORDING IDENTIFICATION NUMBERS OF BACKSCATTERED ELECTRONS
S1 = 123457
S2 = 325017
S3=.56791243

C** S1, S2, AND S3 ARE RANDOM NUMBER GENERATOR SEEDS
C** ALL RANDOM NUMBER GENERATOR SEEDS MUST BE ODD
C** S1, S2, AND S3 ARE DOUBLE PRECISION
IPA=1
ITP=1

C** IPA AND ITP ARE RANDOM NUMBER COUNTERS
C** USED TO CHECK NUMBER OF RANDOM NUMBERS USED OUT OF VECTOR
CS=5.449

C** CS = CONSTANT FOR SCREENING ANGLE
CX=14.4*14.4

C** CX= (CHARGE OF THE ELECTRON IN EV/ANGSTROM)**4
PI=.314159 E 01
CMA=0.6024

C** CMA = AVOGADRO'S NUMBER * (10)**-24
CPI=.2E 01*PI
CE=-CPI*0.6023*14.4*14.4
EIN=20000.

C** EIN = INCIDENT ENERGY OF ELECTRONS
X=0.
Y=0.
Z=0.

C** X, Y, Z = INCIDENT ELECTRON BEAM POSITION
C** ZBX = BOUNDARIES IN Z DIRECTION
12 ZB0=0.
 ZB1=50.
 ZB2=100.
 ZB3=200.
 ZB4=300.
 ZB5=400.
 ZB6=500.
 ZB7=600.
 ZB8=700.
 ZB9=800.
 ZB10=900.
 ZB11=1000.
 ZB12=1100.
ZB13=1150.
ZB14=1200.

C** ZPX = DISTANCE BETWEEN ZB(X-1) AND ZBX BOUNDARY
ZP1=ZB1-ZB0
ZP2=ZB2-ZB1
ZP3=ZB3-ZB2
ZP4=ZB4-ZB3
ZP5=ZB5-ZB4
ZP6=ZB6-ZB5
ZP7=ZB7-ZB6
ZP8=ZB8-ZB7
ZP9=ZB9-ZB8
ZP10=ZB10-ZB9
ZP11=ZB11-ZB10
ZP12=ZB12-ZB11
ZP13=ZB13-ZB12
ZP14=ZB14-ZB13

NPARS=1

C** NPARS = STARTING HISTORY INDEX
NPART=3000

C** NPART = FINISHING HISTORY INDEX
ZCU=29.

C** ZCU = ATOMIC NUMBER OF AN ELEMENT
RHOCU=8.96

C** RHOCU = DENSITY OF AN ELEMENT
ACU=63.546

C** ACU = ATOMIC WEIGHT OF AN ELEMENT
ICU=377.

C** ICU = IONIZATION CONSTANT OF AN ELEMENT
CSCU=CS*ZCU**((.2E0/.3E0)

C** CSCU= CONSTANT FOR SCREENING ANGLE
CXCU=0.2500*PI*CX*ZCU*(ZCU+1.)*CNA*RHOCU/ACU

C** CXCU= CONSTANT FOR CROSS SECTION
CECU=CE*ZCU*RHOCU/ACU

C** CECU= CONSTANT FOR DETERMINING ENERGY LOSS
WRITE(6,63)
63 FORMAT('1','ELECTRON HISTORIES FOLLOW',//)
NP=0
WRITE(6,64)
64 FORMAT('0','RANDOM NUMBER SEEDS')
65 FORMAT('0',3D14.7)
WRITE(6,62)
CALL GGU1(S1,M9AN,RPL)
C** GGU1 IS A INSL SUBROUTINE THAT GENERATES A SET OF PSEUDO RANDOM
C** NUMBERS EQUALLY DISTRIBUTED BETWEEN 0 AND 1
C** IRAN=NUMBER OF RANDOM NUMBERS IN A VECTOR
C** HPL=VECTOR OF PATH LENGTH RANDOM NUMBERS
C** S1, S2, AND S3= RANDOM NUMBER SEEDS THE CALLING VALUE IS
C** REPLACED WITH A NEW VALUE OF THE SEED UPON RETURN FROM GGU1
C** CALL GGU1(S2,M9AN,RAT)
C** RAT=VECTOR OF THETA ANGLE RANDOM NUMBERS
C** CALL GGU1(S3,M9AN,RAP)
C** RAP=VECTOR OF PHI ANGLE RANDOM NUMBERS
DO1NP=NPARS,NPART
C** DO LOOP ON HISTORIES
C** INITIALIZE ELECTRON POSITION, ANGLE, ENERGY, AND TOP LAYER OF
C** MATERIAL
COST=1.0
C** COST=COSINE OF THETA
SINT=0.0
C** SINT=SINE OF THETA
COSP=1.0
C** COSP=COSINE OF PHI
SINP=0.0
C** SINP=SINE OF PHI
C** THETA AND PHI ARE ANGLES OF THE SPHERICAL COORDINATE SYSTEM
ALF=0.0
C** ALF=ALPHA = SCATTERING ANGLE WRT DIRECTION BEFORE COLLISION
C** WRT = WITH RESPECT TO
COSB=0.0
C** COSB=COSINE OF BETA
C** BETA = SECOND SCATTERING ANGLE WRT DIRECTION BEFORE COLLISION
C** WRT = WITH RESPECT TO
NREG=1
**WREG=** THE NUMBER OF THE REGION THE ELECTRON IS IN

**NEVE=-1**

**NEVE=** NUMBER OF EVENTS (COLLISIONS + BOUNDARY CROSSINGS) ELECTRON

**UMDERGOES DURING A TRAJECTORY**

**NCOL=0**

**NCOL=** NUMBER OF COLLISIONS

**NOUT=0**

**NOUT=** TYPE OF OUTER BOUNDARY CROSSING

**E=EIN**

**E=** ENERGY AFTER A COLLISION

**EA=E**

**EA =** ENERGY AT A BOUNDARY

**E AND EA HAVE DIFFERING VALUES ONLY AT BOUNDARIES**

**I=ICU**

**CS=CSCU**

**CE=CSCU**

**CX=CXCU**

**I, CE, CX, AND CS ARE VALUES OF THE PARAMETER IN A SPECIFIC REGION**

**IN THIS CASE, THEY ARE FOR REGION 1 AND MUST BE CHANGED IF ANOTHER**

**MATERIAL IS TO BE USED IN ANOTHER REGION**

**XI=X**

**XI=** X POSITION DURING TRAJECTORY

**XI=Y**

** XI=** Y POSITION DURING TRAJECTORY

**XI=Z**

** XI=** Z POSITION DURING TRAJECTORY

**PRINT RANDOM NUMBER SEEDS ON THE LAST TRAJECTORY**

**IF(NP.LT.NPART)G0TO21**

**WRITE(6,64)**

**WRITE(6,65)S1,S2,S3**

**I=21**

**MAB=0**

**SI=CS/E**

**SI = SCREENING ANGLE**

**SIP=1.+SI**

**SIG=CX/E/E/SI/SIP**

**SIG=RUTHERFORD CROSS SECTION INTEGRATED OVER ALL ANGLES**

**DES=CE ALOG(1.166*E/I)/E**
C** DES= ENERGY LOSS PER UNIT PATH LENGTH  **********
2 RS=RPL(IPA)  
C** RS IS RANDOM NUMBER FOR PATH LENGTH  **********
IPAPA=IPA+1  
IF (IPA.LE.MRAN) GOTO30  
C** CHECK TO SEE IF ALL RANDOM NUMBERS IN THE VECTOR HAVE BEEN USED  **********
C** AND GENERATE MORE IF NECESSARY  **********
CALL GGU1(S1,MRAN,BPL)  
IPA=1  
30 NTYPE=0  
C** NTYPE=0 PATH LENGTH DOES NOT EXCEED LN(0.05)  **********
C** TO FACILITATE EXECUTION PATH LENGTHS GREATER THAN APPROXIMATELY  **********
C** 3* LAMDA ARE NOT USED TO KEEP LN(RS) FROM BLOWING UP  **********
NTYPE=1  
C** NTYPE=1 PATH LENGTH DOES EXCEED LN(0.05)  **********
RS=.05  
8 SIGS=-ALOG(RS)  
C** SIGS= NO. OF MEAN FREE PATHS THE ELECTRON TRAVELS BETWEEN  **********
C** COLLISIONS  **********
S=SIGS/SIG  
C** S = LINEAR DISTANCE  **********
Z0=ZI+S*COST  
C** Z0 = NEW Z COORDINATE  **********
NEVE=NEVE+1  
GOTO20  
7 NEVE=NEVE+1  
WRITE(NW1) E,EA,COST,COSP,XI,YI,ZI,DES,SINP,NP  
C** WRITE DATA ON TAPE IF ELECTRON CROSSES A BOUNDARY  **********
C** E= ENERGY OF ELECTRON AFTER LAST COLLISION  **********
C** EA= ENERGY OF ELECTRON AT THE BOUNDARY  **********
C** COST = COSINE OF THETA  **********
C** COSP= COSINE OF PHI  **********
C** XI=X POSITION OF ELECTRON AT BOUNDARY  **********
C** YI=Y POSITION OF ELECTRON AT BOUNDARY  **********
C** ZI=Z POSITION OF ELECTRON AT BOUNDARY  **********
C** DES=ENERGY LOSS PER UNIT PATH LENGTH IN EV PER ANGSTROM  **********
C** SINP= SINE OF PHI  **********
C** NP= INTEGER IDENTIFYING THIS ELECTRON HISTORY
20 CALL FATE(52,53,54,57)
C** FATE DETERMINES BOUNDARY CROSSINGS
C** NUMBERS IN PARENTHESES INDICATE STATEMENTS THE PROGRAM WILL
C** GO TO NEXT IF TOLD TO RETURN X (WHERE X IS A NUMBER) IN
C** SUBROUTINE FATE
RT=HAT(ITP)
C** RT IS THE RANDOM NUMBER THAT DETERMINES THETA
C0SB=1.-2.*S1*RT/(SIP-RT)
BP=RAP(ITP)
C** RP IS THE RANDOM NUMBER THAT DETERMINES PHI
ITP=ITP+1
IF (ITP.LE.MRAN) GOTO 31
C** CHECK TO SEE IF ALL RANDOM NUMBERS IN THE VECTOR HAVE BEEN USED
C** AND GENERATE MORE IF NECESSARY
CALL GGU1(S2,MRAN,RAT)
CALL GGU1(S3,MRAN,RAP)
ITP=1
C** STATEMENTS 31-73 COMPUTE NEW SCATTERING ANGLES
31 SINB=SQR(1.-COSB*COSB)
ALF=RTI*RP
SINA=SIN(ALF)
COSA=COS(ALF)
XMU=COST*COSB+SINT*SINB*COSA
TMU=SQR(1.-XMU*XMU)
IF (SINT.EQ.0.00) GOTO 70
YYY=(COSB-COST*XMU)/SINT/TMU
XXX=-SINB*SINA/TMU
C** XMU, TMU, XXX, AND YYY ARE INTERMEDIATE VARIABLES
PHI= YYY*COSP-XXX*SIMP
SIMP= XXX*COSP+YYY*SINP
COSP= PHI
GO TO 71
70 COSP=COSA
SIMP=SINA
71 COST=XMU
73 SINT=TMU
NCOL=NCOL+1

C** THE FOLLOWING TERMINATIONS ARE TO SAVE TIME AND ARE BASED ON
OBSERVATIONS OF THE RESULTS OF CALCULATIONS FOR COPPER AT 20 Kev
AND 90 DEGREE INCIDENCE

C** IF (NCOL.GT.400) GOTO1

C** PROGRAM WILL TERMINATE ON THE PARTICULAR TRAJECTORY IF NUMBER OF
COLLISIONS IS GREATER THAN 400

C** IF (E.LT.4000.) GOTO1

C** PROGRAM WILL ALSO TERMINATE IF E IS LESS THAN 4000.

GOTO2

3 NOUT=1

4 NOUT=NOUT+1

C** STATEMENTS 3 AND 4 ARE TERMINATIONS FOR TOP AND BOTTOM BOUNDARY
CROSSINGS

C** NOUT = 1 ELECTRON CROSSED UPPER SURFACE
C** NOUT = 2 ELECTRON CROSSED LOWER SURFACE

WRITE(NW1) E, EA, COST, COSP, XI, YI, ZI, DES, SINP, NP
IP(NOUT.NE.2) GOTO111
WRITE(NW2) E, EA, COST, COSP, XI, YI, ZI, DES, SINP, NP

C** NW2= TAPE FOR STORAGE OF ELECTRON INFORMATION AT BOTTOM BOUNDARY
GOTO1

60 FORMAT(*0.15, 2X, 2E12.5, 2P7.3, 3E12.5, 2P7.3)

62 FORMAT(*0, 4X, NCOL, NEVE, NOUT, NREG, 4X, 'E', 8X, 'EA', 7X, 'COST'

111 WRITE(6, 60) NP, E, EA, COST, COSP, XI, YI, ZI, DES, SINP
1 CONTINUE

C** CLOSE OUT TAPE RECORDS
ENDFILE NW1
REWIND NW1
ENDFILE NW2
REWIND NW2
STOP
END

C** SUBROUTINE FATE DETERMINES IF AN ELECTRON CROSSES A BOUNDARY FROM
ONE REGION TO ANOTHER. IF A BOUNDARY CROSSING OCCURS THIS
SUBROUTINE COMPUTES THE PATH LENGTH TO THE BOUNDARY AND THE
VARIABLE VALUES AT THE BOUNDARY.
IT ALSO SETS THE MATERIAL DEPENDENT PARAMETERS FOR THE MATERIAL TO BE ENCOUNTERED IN THE NEXT REGION.

IT ALSO COMPUTES THE REMAINDER OF THE PATH LENGTH THAT THE ELECTRON MUST TRAVEL IN THE NEXT REGION.

IF NO BOUNDARY IS ENCOUNTERED THEN THE ROUTINE COMPUTES THE NEW POSITION, ENERGY AND ENERGY LOSS PER UNIT PATH LENGTH.

FOR EVERY GEOMETRY TO BE STUDIED A DIFFERENT SUBROUTINE PATE MUST BE USED.

THIS PATE SUBROUTINE HAS 1/4 Z BOUNDARIES TO CHECK.

SUBROUTINE IRATE(*,*, *, *)
REAL*4 X,IAL
COMMON NREG, Z0, ZB4, ZB3, ZB2, ZB1, ZB0, NAB, ZI, XI, S, SINT, COSP, YI, SINP, 
1E, DES, SI, CS, SJP, SIG, CD, CE, X, NTYPE, NOUT, EA, CECU, CECU, CSCU, ICU, SIGS, 
1COST, CX, ZP1, ZP2, ZP3, ZP4, ZB5, ZP5, ZB6, ZP6, ZB7, ZB8, ZB9, ZB10, ZP7, ZP8, 
2ZP9, ZP10, ZP11, ZP12, ZP13, ZP14, NP, NW1
COMMON ZB11, ZB12, ZB13, ZB14

STATEMENTS 1 THROUGH 13 CHECK TO SEE IF ELECTRON CROSSES A BOUNDARY.

GOTO (1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13) , NREG

Z1 = Z0 - ZB13
Z2 = Z0 - ZB14
M = (Z1 + Z2) / ZP14
IF (M) 1413, 100, 1415

1 Z1 = Z0 - ZB0
Z2 = Z0 - ZB1
M = (Z1 + Z2) / ZP1
IF (M) 110, 100, 112

2 Z1 = Z0 - ZB1
Z2 = Z0 - ZB2
M = (Z1 + Z2) / ZP2
IF (M) 121, 100, 123

3 Z1 = Z0 - ZB2
Z2 = Z0 - ZB3
M = (Z1 + Z2) / ZP3
IF (M) 132, 100, 134

4 Z1 = Z0 - ZB3

Z2 = Z0 - ZB1
M = (Z1 + Z2) / ZP1
IF (M) 110, 100, 112

GOTO (1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13) , NREG
\[ Z_2 = Z_0 - Z_{B4} \]
\[ H = \frac{Z_1 + Z_2}{Z_{P4}} \]
\[ \text{IF (M) 143, 100, 145} \]

5 \[ Z_1 = Z_0 - Z_{B4} \]
\[ Z_2 = Z_0 - Z_{B5} \]
\[ M = \frac{Z_1 + Z_2}{Z_{P5}} \]
\[ \text{IF (M) 154, 100, 156} \]

6 \[ Z_1 = Z_0 - Z_{B5} \]
\[ Z_2 = Z_0 - Z_{B6} \]
\[ M = \frac{Z_1 + Z_2}{Z_{P6}} \]
\[ \text{IF (M) 165, 100, 167} \]

7 \[ Z_1 = Z_0 - Z_{B6} \]
\[ Z_2 = Z_0 - Z_{B7} \]
\[ M = \frac{Z_1 + Z_2}{Z_{P7}} \]
\[ \text{IF (M) 176, 100, 178} \]

C** NUMBERS ON IF STATEMENTS REFER TO WHAT BOUNDARY WAS CROSSED
C** 178 REFERS TO A CROSSING OF ZB7 FROM REGION 7 TO REGION 8
C** 187 REFERS TO A CROSSING OF ZB7 FROM REGION 8 TO REGION 7
C** 198 REFERS TO A CROSSING OF ZB8 FROM REGION 8 TO REGION 7
C** 209 REFERS TO A CROSSING FROM REGION 10 TO REGION 9

8 \[ Z_1 = Z_0 - Z_{B7} \]
\[ Z_2 = Z_0 - Z_{B8} \]
\[ M = \frac{Z_1 + Z_2}{Z_{P8}} \]
\[ \text{IF (M) 187, 100, 189} \]

9 \[ Z_1 = Z_0 - Z_{B8} \]
\[ Z_2 = Z_0 - Z_{B9} \]
\[ M = \frac{Z_1 + Z_2}{Z_{P9}} \]
\[ \text{IF (M) 198, 100, 190} \]

10 \[ Z_1 = Z_0 - Z_{B9} \]
\[ Z_2 = Z_0 - Z_{B10} \]
\[ M = \frac{Z_1 + Z_2}{Z_{P10}} \]
\[ \text{IF (M) 209, 100, 211} \]

C** 1109 REFERS TO A CROSSING FROM REGION 10 TO REGION 9

11 \[ Z_1 = Z_0 - Z_{B10} \]
\[ Z_2 = Z_0 - Z_{B11} \]
\[ M = \frac{Z_1 + Z_2}{Z_{P11}} \]
\[ \text{IF (M) 1110, 100, 1112} \]

12 \[ Z_1 = Z_0 - Z_{B11} \]
\[ Z_2 = Z_0 - Z_{B12} \]
M = (Z1 + Z2) / ZP12
IF(M) 1211, 100, 1213
13 Z1 = Z0 - ZB12
Z2 = Z0 - ZB13
M = (Z1 + Z2) / ZP13
IF(M) 1312, 100, 1314
100 ZI = Z0
C** ROUTINE GOES TO STATEMENT 100 IF NO BOUNDARY IS CROSSED
C** THIS COMPUTES A NEW ENERGY, POSITION, AND ENERGY LOSS PER UNIT
C** PATH LENGTH IN THE REGION
XI = XI + S * SINT * COSP
YI = YI + S * SINT * SINP
E = EA + DES * S
EA = E
SI = CS / E
SIP = SI + 1.
SIG = CX / E / E / SI / SIP
DES = CE * ALOG(1.166 * E / I) / E
IF (ZI .GT. 100.) GOTO 20
WRITE (NW1) E, EA, COST, COSP, XI, YI, DES, SINP, NP
C** WRITE ON TAPE FOR USE IN SECONDARY ELECTRON PRODUCTION PROGRAM
20 IF (NTYPE .EQ. 1) RETURN 1
RETURN
1415 S = (ZB14 - ZI) * S / (Z0 - ZI)
C** IN THIS CASE STATEMENT 1415 IS FOR CROSSING THE LOWER BOUNDARY
C** UPDATE POSITION, ENERGY, AND ENERGY DEPENDENT PARAMETERS
ZI = ZB14
XI = XI + S * SINT * COSP
YI = YI + S * SINT * SINP
EA = EA + S * DES
RETURN 2
110 S = (ZI - ZBO) * S / (Z0 - ZI)
C** STATEMENT 110 IS FOR CROSSING THE UPPER BOUNDARY
C** UPDATE POSITION, ENERGY, AND ENERGY DEPENDENT PARAMETERS
ZI = ZBO
XI = XI + S * SINT * COSP
YI = YI + S * SINT * SINP
EA = EA + S * DES
RETURN 3

C** STATEMENTS 1413 THROUGH 112 CALCULATE THE PATH LENGTH THE
ELECTRON TRAVELS TO THE BOUNDARY

1413 S = (ZI - ZB13) * S / (ZI - Z0)
ZI = ZB13
NREG = 13
GOTO 106

1314 S = (ZB13 - ZI) * S / (Z0 - ZI)
ZI = ZB13
NREG = 14
GOTO 106

1312 S = (ZI - ZB12) * S / (ZI - Z0)
ZI = ZB12
NREG = 12
GOTO 106

1213 S = (ZB12 - ZI) * S / (Z0 - ZI)
ZI = ZB12
NREG = 13
GOTO 106

1211 S = (ZI - ZB11) * S / (ZI - Z0)
ZI = ZB11
NREG = 11
GOTO 106

1112 S = (ZB11 - ZI) * S / (Z0 - ZI)
ZI = ZB11
NREG = 12
GOTO 106

1110 S = (ZI - ZB10) * S / (ZI - Z0)
ZI = ZB10
NREG = 10
GOTO 106

1011 S = (ZB10 - ZI) * S / (Z0 - ZI)
ZI = ZB10
NREG = 11
GOTO 106

1109 S = (ZI - ZB9) * S / (ZI - Z0)
ZI = ZB9
NREG = 9
GOTO 106

910 S = (ZB9 - ZI) * S / (ZO - ZI)
ZI = ZB9
NREG = 10
GOTO 106

198 S = (ZI - ZB8) * S / (ZI - Z0)
ZI = ZB8
NREG = 8
GOTO 106

189 S = (ZB8 - ZI) * S / (Z0 - ZI)
ZI = ZB8
NREG = 9
GOTO 106

178 S = (ZB7 - ZI) * S / (Z0 - ZI)
ZI = ZB7
NREG = 8
GOTO 106

187 S = (ZI - ZB7) * S / (ZI - Z0)
ZI = ZB7
NREG = 7
GOTO 106

167 S = (ZB6 - ZI) * S / (Z0 - ZI)
ZI = ZB6
NREG = 7
GOTO 106

176 S = (ZI - ZB6) * S / (ZI - Z0)
ZI = ZB6
NREG = 6
GOTO 106

165 S = (ZI - ZB5) * S / (ZI - Z0)
ZI = ZB5
NREG = 5
GOTO 105

156 S = (ZB5 - ZI) * S / (Z0 - ZI)
ZI = ZB5
NB EG=6
GOTO 106

154 S = (ZI - ZB4) * S / (ZI - Z0)
    ZI = ZB4
    NREG = 4
    GOTO 104

145 S = (ZB4 - ZI) * S / (Z0 - ZI)
    ZI = ZB4
    NREG = 5
    GOTO 105

134 S = (ZB3 - ZI) * S / (Z0 - ZI)
    ZI = ZB3
    NREG = 4
    GOTO 104

143 S = (ZI - ZB3) * S / (ZI - Z0)
    ZI = ZB3
    NREG = 3
    GOTO 103

123 S = (ZB2 - ZI) * S / (Z0 - ZI)
    ZI = ZB2
    NREG = 3
    GOTO 103

132 S = (ZI - ZB2) * S / (ZI - Z0)
    ZI = ZB2
    NREG = 2
    GOTO 102

121 S = (ZI - ZB1) * S / (ZI - Z0)
    ZI = ZB1
    NREG = 1
    GOTO 101

112 S = (ZB1 - ZI) * S / (Z0 - ZI)
    ZI = ZB1
    NREG = 2

103 CONTINUE

C** NUMBERS 10X ARE CONTINUATION STATEMENTS FOR THE XTH REGION FOR ********
C** CHANGE OF MATERIALS ********
C** IF DIFFERENT MATERIALS ARE TO BE USED IN SEPERATE REGIONS THEN ********
INSERT MATERIAL DEPENDENT PARAMETERS AFTER PROPER CONTINUATION

STATEMENT

CONTINUE
CONTINUE
CONTINUE
CONTINUE

AFTER 102 INSERT PROPER MATERIAL PARAMETERS FOR REGION 2

IN THIS PARTICULAR CASE ONLY ONE MATERIAL IS BEING USED

COMPUTE ENERGY AND X Y POSITION ON BOUNDARY

EA=EA+S*DES
XI=XI+S*SINT*COSP
YI=YI+S*SINT*SINP
CE=CECU
CX=CXCU
CS=CSCU
I=ICU

PURPOSELY USE E RATHER THAN EA IN THE FOLLOWING SO THAT IF THE
SAME MATERIAL IS USED IN BOTH REGIONS THE FINAL POSITION WILL BE
IDENTICAL TO THAT IF BOUNDARY WAS NOT PRESENT

SIGS=SIGS*SIG*S
SI=CS/E
SIP=1.+SI
SIG=CX/E/E/SI/SIP
DES=CE*ALOG(1.166*E/I)/E

COMPUTE PATH LENGTH THAT REMAINS TO BE TRAVELED BY THE ELECTRON
IN THE NEW REGION BEFORE IT UNDERGOES A COLLISION

S=SIGS/SIG
NAB=NAB+1
Z0=ZI+S*COST
RETURN 4
END
Multiple scattering data program

Start

Enter initial energy of multiple scattering, number of collisions per multiple scattering step, and the atomic number, atomic weight, material density, and ionization constant for the element for which the multiple scattering data is to be calculated

Enter number of angles for which the multiple scattering cross section is to be evaluated at each angular interval

Enter starting angle for each set of angles for which the multiple scattering cross section is to be evaluated

Enter degree of convergence desired in the expansion to determine the value of the integral cross section and the maximum number of terms to be used in the expansion

Compute energy, step length, and energy loss per unit path length for the multiple scattering steps

Record these values on magnetic tape

Calculate the polar scattering angles to be used in the evaluation of the multiple scattering angular cross section

Calculate the first through the maximum number of expansion terms order Legendre polynomials of the first kind for the cosine of these angles

Figure A2. Logic diagram of the multiple scattering data program
Have the calculations of the angular scattering cross sections been completed for all multiple scattering steps?

No

Calculate the values of $k_i$ for this multiple scattering step energy

Has the integral cross section for the polar angle been calculated for all angles?

No

Calculate the first term in the expansion for the integral cross section for the next angle

Calculate the next term in the expansion for the integral cross section for this angle

Has the integral cross section converged to the desired degree of accuracy?

No

Yes

Stop

Yes

Figure A2 (Continued)
Figure A2 (Continued)
MULTIPLE SCATTERING MONTE CARLO DATA PROGRAM

IMPLICIT REAL*8(A-H,O-Z)
REAL*4XM,VALU,TERMS,THMT,THET4,FT,FM,F,SF,SG,ARG,VAL,SH,SL,ENE

DIMENSION E(30),DELS(30),P(60),PL(108,60),F(108),FT(108),
1KTER(108),TERMS(91),THMT(108),NTH(3),MTH(3),ARG(20),VAL(20),DE(3),
2DIRECTION ENE(3)

DATA PI/3.141593/,AVN/0.6023/,SE2/14.4/

C++ AVN=AVOGADO'S NUMBER IN ATOMS PER (ANGSTROM)^3
C++ SE2=ELECTRON CHARGE IN ELECTRON VOLTS/ANGSTROM

NE=9
NRR=10

C++ NR AND NRR ARE UNIT NUMBERS FOR RECORDING INFORMATION ONTO
C++ MAGNETIC TAPE

E0=18900.

C++ E0=INITIAL ENERGY OF MULTIPLE SCATTERING
PE=22.61
C++ PE=NUMBER OF ELASTIC SCATTERING COLLISIONS PER MULTIPLE SCATTERING

C++ STEP
Z=29.

C++ Z=ATOMIC NUMBER
AN=63.546
C++ AN=ATOMIC MASS
RO=8.96
C++ RO=DENSITY
CION = 377.

C++ CION=IONIZATION CONSTANT OBTAINED FROM DUNCOMB AND REED
CK=5.449
C++ CK=CONSTANT FOR SCREENING ANGLE USING NIGAM'S EXPRESSION

NTH(1)=58
C++ NTH(1)=THE NUMBER OF ANGLES TO BE EVALUATED AT EVERY 1 DEGREE
NTH(2)=26
C++ NTH(2)=THE NUMBER OF ANGLES TO BE EVALUATED AT EVERY 2 DEGREES
NTH(3)=24
C** NTH(3) = THE NUMBER OF ANGLES TO BE EVALUATED AT EVERY 3 DEGREES
MTH(1)=-1
C** MTH(1) = MINIMUM VALUE OF BETA MINUS ONE FOR THE FIRST SET OF
ANGLES
MTH(2)=56
C** MTH(2) = MINIMUM VALUE OF BETA MINUS TWO FOR THE SECOND SET OF
ANGLES
MTH(3)=108
C** MTH(3) = MINIMUM VALUE OF BETA MINUS THREE FOR THE THIRD SET OF
ANGLES
C** EPSI1=0.0001
C** EPSI1= DESIRED ACCURACY OF CROSS SECTION EXPANSION
INTERMS=56
MXTRM=56
C** INTERMS=MXTRM=MAXIMUM NUMBER OF TERMS USED IN EXPANSION TO
Determine THE VALUE OF THE CROSS SECTION
AND=RO*AVN/AN
C** AND = NUMBER OF NUCLEI PER UNIT VOLUME
V11=AN*PE*1.0E-01/(3.*Z(4./3.)*RD)
C** V11 USED TO DETERMINE STEP LENGTH BY NUMBER OF SCATTERING
C** EVENTS CRITERION
E(1)=E0
C** E(1) = INITIAL ENERGY OF ELECTRON
DELS(1)=V11*E0
DE(25)=0.
V2=2.*PI*AND*Z*SE2*SE2
V3=(SQRT (EXP (1.0)/2.0) /CION)
V4=V2*(Z+1.)/4.
V5=CK*Z**(2./3.)
C** V1, V2, V3, V4, AND V5 ARE INTERMEDIATE VARIABLES USED IN THE
CALCULATIONS
C** SS=DELS(1)
DO 1 I=1,24
C** THIS LOOP DETERMINES STEP LENGTH AND ENERGY LOSS AND THE ENERGY AT
BEGINNING AND END OF EACH STEP LENGTH
DEDS=-DLOG (E(I)*V3)*V2/E(I)
DE(I)=DEDS

161
DE(I) = ENERGY LOSS PER UNIT PATH LENGTH VECTOR

E(I+1) = E(I) + DEDS*DELS(I)

E(I) = ENERGY VECTOR

E(2) = ENERGY BEFORE FIRST COLLISION

E(3) = ENERGY BEFORE SECOND COLLISION

DELS(I+1) = V11*E(I+1)

DELS(I) = STEP LENGTH VECTOR

SS = SS + DELS(I+1)

SS = TOTAL DISTANCE TRAVELED BY THE ELECTRON

CONTINUE

WRITE THESE VECTORS ON TAPE

WRITE(NR) E

WRITE(NR) DELS

ENDFILE NR

REWIND NR

ME = 25

NT = NUMBER OF TERMS + 1

NT = NUMBER OF TERMS IN LEGENDRE POLYNOMIAL EXPANSION

I J = 0

DO 211 = 1, 3

LOOP ENDING WITH STATEMENT NO. 2 DETERMINES ANGLES TO BE USED

IN THE CALCULATION OF THE SCATTERING CROSS SECTION AND VALUE OF

LEGENDRE POLYNOMIAL EXPANSION FOR COSINE(\beta)

INCTH = II

INCTH = AMOUNT TO INCREMENT \beta BY EACH TIME

NTHETA = NTH(IJ)

NTHETA = NUMBER OF TIMES TO INCREMENT \beta

MINTH = MTH(IJ)

MINTH = MINIMUM VALUE OF \beta MINUS THE FIRST INCREMENT

DO 211 = 1, NTHETA

THETA = IJ*INCTH + MINTH

THETA = THETA*PI/180.

IJ = IJ + 1

THETA4 = THETA

THETA4 = SINGLE PRECISION \beta VARIABLE
TM(1J) = THETA4
COST = DCOS(THETA)
CALL DPEP (? ,COST, NT)
DO2J=1,NT
  PL(1J, J) = P(J)
C** PL(1J, J) = THE JTH LEGENDRE POLYNOMIAL FOR THE IJ VALUE OF BETA
NTETHA=108
C** NTHETA IS THE TOTAL NUMBER OF BETA VALUES
DO3I=1,KE
C** THIS LOOP ENDING WITH STATEMENT NO. 3 COMPUTES THE ANGULAR CROSS
C** SECTION FOR ME ENERGIES AND STEP LENGTHS
DEL=DELS(I)
EP=E(I)
BETA=V5/EP
C** BETA= ACTUAL VALUE OF SCREENING ANGLE
VE1=V4/EP**2
VE2=1.+2.*BETA
VE3=1./(1.+BETA)
C** VE1, VE2, AND, VE3 ARE INTERMEDIATE VARIABLES
P(1)=0.0
X=0.0
Y=DLLOG (1.+1./BETA)-VE3
P(2)=Y
MXTR=MXTTR-1
DO4J=2,4MXTR
C** LOOP ENDING IN STATEMENT NO. 4 COMPUTES THE VALUE OF KAPPA SUB I
C** USING AN EXPANSION OF LEGENDRE POLYNOMIALS
XJ=J-1
XJ=1./XJ
XJ1=2.+XJ
Z=XJ1*VE2*Y-(1.+XJ)*X-XJ1*VE3
P(J+1)=Z
C** P(J) = VALUE OF THE JTH TERM IN THE EXPANSION OF KAPPA SUB I FOR
C** THE ITH ENERGY AND PATH LENGTH
X=Y
Y=Z
DO5J=1,NTHETA
LOOP ENDING IN STATEMENT NO. 5 COMPUTES THE DIFFERENTIAL AND INTEGRAL CROSS SECTIONS AS A FUNCTION OF BETA

\[ F_{TH} = 0.5 \]
\[ F_{THH} = 0.5 \times (1 - P_L(J, 2)) \]
\[ N_S = 2 \]
\[ N_{STP} = 8 \]
\[ D07L = 1, 7 \]

NS AND NSTP ARE CONSTANTS USED IN DO LOOP 6 SO TO GET THE RIGHT VALUES OF PL(J,K)

\[ D06K = N_S, N_{STP} \]
\[ V_K1 = 2 \times K - 1 \]
\[ V_K1 = V_K1 \times 0.5 \]
\[ G_L = DEXP(-V_B1 \times P(K) \times D_1) \]
\[ F_{TH1} = F_{TH} \]
\[ F_{TH2} = F_{THH} \]
\[ F_{THH} = F_{THH} + G_L \times (P_L(J, K-1) - P_L(J, K+1)) \times 0.5 \]
\[ F_{TH} = F_{TH} + G_L \times V_K1 \times P_L(J, K) \]

\[ F_{THH} = 2 \pi \times \text{THE INTEGRAL FROM ZERO TO BETA OF } P(BETA) \times \text{SIN}(BETA) \times DBETA \]
\[ F_{TH} = 2 \pi \times P(BETA) \]

CON = DABS(FTH1 - FTH)

IF(CON .LE. EPSI 1) GOTO 8

CONVERGENCE IS CHECKED ON INTEGRAL CROSS SECTION VALUE AFTER EVERY 7 TERMS IN THE EXPANSION

MAXIMUM NUMBER OF TERMS IS 56

\[ N_S = L \times 8 + 1 \]
\[ N_{STP} = (L + 1) \times 8 \]
\[ K_{TER}(J) = K \]

KTER(J) = NUMBER OF TERMS USED IN EXPANSION FOR ANGLE J

FT(J) = FTHH

FT(J) = INTEGRAL SCATTERING CROSS SECTION FOR ANGLE J

F(J) = FTH

F(J) = DIFFERENTIAL SCATTERING CROSS SECTION FOR ANGLE J

THIS IS FOR PRINTED OUTPUT ONLY

WRITE (6, 100)
WRITE (6, 102)
WRITE(6,101)8(1),E(I+1),DELS(I)
DO30IK=2,90

THE LOOP ENDING WITH STATEMENT NO. 30 IS USED TO PUT THE ANGULAR CROSS SECTION IN A TABULAR FORM WITH EQUAL INCREMENTAL VALUES OF THE CROSS SECTION AND THE CORRESPONDING ANGULAR VALUE

THE PURPOSE OF THIS IS THAT DURING EXECUTION OF THE MONTE CARLO PROGRAM A RANDOM NUMBER IS GENERATED AND AN INTERPOLATION IS DONE USING THE TABLE TO DETERMINE THE SCATTERING ANGLE

XI=IK

XM=(XI-1.)/90.

XM= THE VALUE OF THE INTEGRAL SCATTERING CROSS SECTION FOR WHICH A CORRESPONDING VALUE OF BETA IS TO BE FOUND BY INTERPOLATION

CALL ATSM(XM,FT,THMT,108,1,ARG,VAL,10)

ATSM IS A IBM SSP SUBROUTINE

IT OBTAINS THE VALUES OF THE CROSS SECTION AND CORRESPONDING ANGLES NEAR THE VALUE XM FOR WHICH A VALUE OF BETA IS TO BE DETERMINED

XM=SEARCH ARGUMENT

FT=VECTOR OF ARGUMENT VALUES (CROSS SECTION VALUES)

THMT=VECTOR OF FUNCTION VALUES (BETA)

108 = Dimension of FT and THMT

1=NUMBER OF COLUMNS IN THMT

ARG=RESULTING VECTOR OF SELECTED AND ORDERED ARGUMENT VALUES

VAL=RESULTING VECTOR OF FUNCTION VALUES

10=NUMBER OF MEMBERS OF ARG AND VAL

CALL ALI(XM,ARG,VAL,VALU,10,0.00010,IER)

ALI DOES THE INTERPOLATION FROM ATSM VALUES

IT IS AN IBM SSP SUBROUTINE

XM=ARGUMENT VALUE

ARG AND VAL= SEE ATSM

VALU= RESULTING INTERPOLATION FUNCTION VALUE

10 = Dimension of ARG AND VAL

0.00010= UPPER BOUND FOR THE ABSOLUTE ERROR IN INTERPOLATION

IER=ERROR PARAMETER

IER=1 IMPOSSIBLE TO REACH REQUIRED ACCURACY BECAUSE OF Rounding

IER=2 REQUIRED ACCURACY COULD NOT BE REACHED BECAUSE TABLE WAS TOO SMALL. INCREASE NUMBER OF MEMBERS IN THE TABLE
IER=3  TWO ARGUMENT VALUES IN VECTOR ARE IDENTICAL
NUMBER OF ARGUMENT VALUES USED IN INTERPOLATION WAS DETERMINED BY TRYING VARIOUS NUMBER OF TERMS AND COMPARING THE MAXIMUM UPPER ERROR BOUND THAT WAS ACHIEVEABLE

KTER (IK) = IER
30 TERMS (IK) = VALU
TERMS (1) = 0.
TERMS (91) = PI

THE VECTOR TERMS (I) CONTAINS THE ANGULAR VALUES THAT CORRESPOND TO
91 EVENLY DISTRIBUTED CROSS SECTION VALUES BETWEEN 0 AND 1

USING THIS TECHNIQUE ONLY THE ANGULAR VALUES NEED TO BE STORED ON TAPE

WRITE (NRR) TERMS
CONTINUE
ENDFILE NRR
REWIND NRR
GOTO 1001

100 FORMAT (0*, //, 4X, 'E IN', 7X, 'E OUT', 7X, 'DELTA S')
101 FORMAT (0*, 3D14.7, I5, /)
102 FORMAT (0*, 4X, 'EV', 10X, 'EV', 10X, 'ANG')
103 FORMAT (0*, 2X, 'THETA', 2X, 'F (THETA)', 2X, 'FT (THETA)', 2X, 'TERMS')
104 FORMAT (0*, 'I5, 2X, 2E14.7, 2X, 15, 2X, 2E14.7, F10.5, E12.5, F10.5)
105 FORMAT (0*, 'THICKNESS TO SMALL FOR MULTIPLE SCATTERING')
106 FORMAT (0*, '4D14.7')
107 FORMAT (0*, F12.8, I5)
1000 WRITE (6, 105)
1001 STOP
END

SUBROUTINE DPLEP (Y, X, N)

SUBROUTINE DPLEP EVALUATES LEGENDRE POLYNOMIALS
IMPLICIT REAL*8 (A-H, O-Z)
DIMENSION Y (80)

Y IS THE VECTOR OF LEGENDRE POLYNOMIALS OF ORDER 0 TO N-1
X IS THE ARGUMENT OF THE LEGENDRE POLYNOMIALS
N IS THE ORDER OF THE LEGENDRE POLYNOMIAL

Y (1) = 1.
DO
Y (2) = X
DO4 I = 2, N
G = X * Y(I)
Y(I+1) = G - Y(I-1) + G - (G - Y(I-1)) / DFLOAT(I)
RETURN
END
Combined single and multiple scattering theory Monte Carlo program

Start

Read in random number seeds

Form random number vectors

Enter boundary positions

Enter or calculate the distance between boundaries

Enter incident energy, number of trajectories, incident beam position, and the atomic number, atomic weight, material density, and ionization constant for each element used in the calculations

Calculate constants for screening angle, cross section, and energy loss equations

Read in vectors of energy, path length, and energy loss per unit path length for each multiple scattering step from magnetic tape

Read in vector of the values of the polar scattering angle that correspond to the 91 equally distributed values of the scattering cross section for each multiple scattering collision from magnetic tape

Calculate the sum of the remaining multiple scattering path lengths for each multiple scattering step

Figure A3. Logic diagram of the combined single and multiple scattering theory Monte Carlo program
Initialize electron energy, position, energy loss per unit path length, and incident angle of the electron beam

Enter the energy at which the electron history is to be terminated

Set the initial multiple scattering energy to the first energy in the multiple scattering energy vector

Enter single scattering portion of the program with the electron energy, position, direction of travel, and region where the electron is located

Calculate macroscopic cross section or mean free path and energy loss per unit path length

Calculate path length the electron travels between elastic collisions

Calculate the Z coordinate that corresponds to the electron traveling this path length

Figure A3 (Continued)
Does the electron cross a boundary?

Yes → 2

No →

Calculate the new electron position, energy, energy loss per unit path length and mean free path

Store electron energy, position, direction of travel, and energy loss per unit path length in the core

Is the electron out of the single scattering region?

Yes → 3

No →

Is the electron energy less than the lower energy limit?

Yes → 7

No →

Calculate the polar, β, and azimuthal, α, scattering angles with respect to the electron's previous direction of travel

3

Figure A3 (Continued)
Figure A3 (Continued)
Is the starting multiple scattering energy less than the present electron energy?

Obtain the next lowest energy in the multiple scattering energy vector

Is the electron energy greater than the starting multiple scattering energy?

Calculate all electron parameters to correspond to this multiple scattering energy

Write stored history on magnetic tape

Figure A3 (Continued)
Enter multiple scattering portion of the program with the new electron parameters.

Determine what percentage of the path length the electron should travel before undergoing an elastic collision.

Calculate the corresponding Z coordinate.

Does the electron return to the single scattering region?

Yes → Calculate other electron coordinates and energy.

No → Calculate the polar, $\beta$, scattering angle by generating a value of the cross section and determining the value of $\beta$ from the tabulated values of the scattering angles.

Calculate the azimuthal, $\alpha$, angle and calculate the value of $\theta$ and $\phi$ the scattering angles with respect to the coordinate system of the electron beam and specimen.

Calculate the rest of the multiple scattering path length.

Figure A3 (Continued)
Does the electron return to the single scattering region? 

Yes → 14

No

Calculate the X and Y coordinates and the electron energy

Is the distance to the specimen surface greater than the remaining multiple scattering path lengths? 

Yes → 7

No

Calculate the electron parameters at the boundary where the electron enters the single scattering region

14

12

16

Has the vector of multiple scattering energies been exhausted? 

Yes → 7

No → 17

Figure A3 (Continued)
**COMBINED SINGLE AND MULTIPLE SCATTERING THEORY MONTE CARLO PROGRAM**

**REAL** S1, S2, S3
**REAL** 4 I, IAL, IU, LAMG
**REAL** 8 EE

**DIMENSION** EE(25), EN(25), DELS(25), DE(25), AMS(25, 91), A(91),
TS(9), TLEF(25), WRT(9, 250), RPL(2500), RAT(2500), RAP(2500), HPW(160)

**COMMON** NREG, ZB4, ZB3, ZB2, ZB1, ZB0, NAB, ZI, XI, S, SINT, COSP, YI, SINP,
1E, DES, SI, CS, SIP, SIG, CD, CE, I, NTYPE, NOUT, EA, CEAL, CXAL, IAL, SIGS,
2COST, CX, ZP1, ZP2, ZP3, ZP4, EMS, ESTOP, ISDST, ISDTI, ISDP1, ZMS, COSB, TPI,
3NCOL, IU, CSU, CXU, CEU, EM, LAMG, NC, NP, IE,
4ZB5, ZP5, ZB6, ZP6, ZB7, ZP7, ZB8, ZP8, ZB9, ZP9, ZB10, ZP10, ZB11, ZP11,
5ZB12, ZP12, ZB13, ZP13, ZB14, ZP14

**COMMON**/CMS/AMS, DELS, DE, TLEF, ID
**COMMON**/RNDM/S1, S2, S3, RAT, RAP, RPL, ITP, MRAN

**COMMON**/WRSP/WRT, NPW, NRPR

500 **MRAN** = 2500

**MRAN** = SIZE OF RANDOM NUMBER VECTOR
**NRPR** = COUNTER FOR RECORDING IDENTIFICATION NUMBERS OF
**BACKSCATTERED ELECTRONS**
**READ** (5, 202) S1, S2, S3

**S1, S2, AND S3 ARE RANDOM NUMBER GENERATOR SEEDS**
**ALL RANDOM NUMBER GENERATOR SEEDS MUST BE ODD $$$$**

**S1, S2, AND S3 ARE DOUBLE PRECISION**

202 **FORMAT** (3D14.7)
**CALL** GGU1(S1, MRAN, RPL)
**CALL** GGU1(S2, MRAN, RAT)
**CALL** GGU1(S3, MRAN, RAP)

**GGU1 IS A IMSL SUBROUTINE THAT GENERATES A SET OF PSEUDO RANDOM**
**NUMBERS EQUALLY DISTRIBUTED BETWEEN 0 AND 1**

**MRAN** = NUMBER OF RANDOM NUMBERS IN A VECTOR
**S1, S2, AND S3 ARE RANDOM NUMBER SEEDS THE CALLING VALUE IS**
**REPLACED WITH A NEW VALUE OF THE SEED UPON RETURN FROM 3GU1**

**BPL=VECTOR OF PATH LENGTH RANDOM NUMBERS**

**BAT=VECTOR OF BETA ANGLE RANDOM NUMBERS**

**RAP=VECTOR OF ALPHA ANGLE RANDOM NUMBERS**

IPL=1

ITP=1

**IPA AND ITP ARE RANDOM NUMBER COUNTERS**

**USED TO CHECK NUMBER OF RANDOM NUMBERS USED OUT OF VECTOR**

CS=5.449

**CS=CONSTANT FOR SCREENING ANGLE**

CX=14.4*14.4

**CX= (CHARGE OF THE ELECTRON IN EV/ANGSTROM) **

PI=.314159E 01

CNA=0.6024

**CNA= AVOGADRO'S NUMBER * (10)**

TPI=.2E 01*PI

CE=TPI*0.6023*14.4*14.4

**ZBX= BOUNDARY IN THE Z DIRECTION**

ZB0=0.0

ZB1=50.

ZB2=100.

ZB3=200.

ZB4=300.

ZB5=400.

ZB6=500.

ZB7=600.

ZB8=700.

ZB9=800.

ZB10=900.

ZB11=1000.

ZB12=1100.

ZB13=1150.

ZB14=1200.

**ZPX= DISTANCE BETWEEN ZBX AND ZB(X-1) BOUNDARIES**

ZP1=ZB1-ZB0

ZP2=ZB2-ZB1

ZP3=ZB3-ZB2
ZP4=100.
ZP5=100.
ZP6=100.
ZP7=100.
ZP8=100.
ZP9=100.
ZP10=100.
ZP11=100.
ZP12=100.
ZP13=50.
ZP14=50.
NMST=25
C** NMST = NUMBER OF MULTIPLE SCATTERING STEPS
NPARS=1
C** NPARS = STARTING ELECTRON ID NUMBER
NPART=10000
C** NPART = ENDING ELECTRON ID NUMBER
EO=20000.
C** EO = INCIDENT ELECTRON ENERGY
X=0.0
Y=0.0
Z=0.0
C** X, Y, Z, = INCIDENT BEAM POSITION
ZAL=29.
C** ZAL= ATOMIC NUMBER OF ELEMENT
RHOAL=8.96
C** RHOAL = DENSITY OF ELEMENT
AAL=63.546
C** AAL = ATOMIC WEIGHT OF ELEMENT
IAL=377.
C** IAL = IONIZATION CONSTANT FOR ELEMENT
CSAL=CS*ZAL**(.2E0/.3E0)
C** CSAL= CONSTANT FOR SCREENING ANGLE
CXAL=0.2500*PI*CX*ZAL*(ZAL+1.)*CNA*RHOAL/AAL
C** CXAL= CONSTANT FOR CROSS SECTION
CEAL=CE*ZAL*RHOAL/AAL
CEAL = CONSTANT FOR DETERMINING ENERGY LOSS

**
NR = 9
NRR = 10

**
MR AND NRR ARE TAPE IDENTIFICATION NUMBERS

**
STATEMENTS DOWN TO 30 ARE TO READ IN THE PARAMETERS FOR THE

**
MULTIPLE SCATTERING MODEL SUBROUTINES

**
THIS PROGRAM IS DESIGNED FOR THE OUTPUT OF THE MULTIPLE SCATTERING

**
DATA PROGRAM FOR 25 MULTIPLE SCATTERING STEPS

**
MR AND NRR ARE NUMBERS FOR THE TAPE JCL FOR FORTRAN INPUT

**
STATEMENTS

**
IC = -1

**
IC = VARIABLE THAT TELLS THE PROGRAM INTO WHICH MATRIX IT IS TO

**
PUT THE INFORMATION IT HAS READ OFF THE TAPE

15 READ (NR, END = 10) EE

**
EE = VECTOR USED TO READ IN PARAMETERS

**
IF (IC) 11, 12, 13

11 DO 14 L = 1, NMST
14 EM (L) = EE (L)

**
EM = THE FIRST VECTOR ON THE TAPE IS THE ENERGY ASSOCIATED WITH

**
EACH MULTIPLE SCATTERING STEP

IC = IC + 1
GOTO 15

12 DO 16 L = 1, NMST
16 DELS (L) = EE (L)

**
DELS = THE SECOND VECTOR IS THE DISTANCE TRAVELED IN EACH MS STEP

**
IC = IC + 1
GOTO 15

13 DO 17 L = 1, NMST
17 DE (L) = EE (L)

**
DE = THE THIRD VECTOR IS THE ENERGY LOSS PER UNIT PATH LENGTH FOR

**
EACH MS STEP

10 L = 1
REWIND NR
20 READ (NRR, END = 18) A
DO 19 J = 1, 91
19 AMS (L, J) = A (J)
L = L + 1
L= (1 TO WNST) = \text{IDENTITY OF EACH MEMBER OF THE SET OF PARAMETERS}  
\text{FOR THE MULTIPLE SCATTERING ROUTINE}  
\text{AMS} = \text{MATRIX OF VALUES OF THE MULTIPLE SCATTERING ANGLES}  
\text{THE 91 VALUES OF THE ANGLES ARE FOR 91 CROSS SECTION VALUES}  
\text{EQUALLY DISTRIBUTED BETWEEN 0 AND 1}  
\text{AMS( L,1) = 0.0 CORRESPONDS TO A CROSS SECTION VALUE OF 0}  
\text{AMS( L,91) = PI CORRESPONDS TO A CROSS SECTION VALUE OF 1}  
GOTO 20

18 \text{REWIND NR}  
TLEF(25) = DELS(25)  
DO93 KI=1,24  
KK=25-KI

93 TLEF( KK) = TLEF( KK+1) + DELS( KK)  
\text{TLEF( KK) = AMOUNT OF MULTIPLE SCATTERING PATH LENGTH LEFT}  
\text{FOR THE KK STEP}  
\text{START LOOP TO RECORD HISTORIES}  
DO1000 NP=NPARS,NPART  
IE=1

C** IE IS THE PARAMETER USED TO IDENTIFY WHICH MEMBER OF THE SET  
C** OF MULTIPLE SCATTERING PARAMETERS SHOULD BE USED FOR THE FIRST  
C** MULTIPLE SCATTERING STEP FOR A GIVEN ELECTRON  
C** NP = ELECTRON IDENTIFICATION NUMBER  
C** PROGRAM CHECKS IF THE NEW ELECTRON ENERGY IS GREATER THAN THE  
C** ENERGY THAT IS AT THE START OF THE MULTIPLE SCATTERING STEP  
C** IF NOT THE PROGRAM THEN STARTS WITH THE NEXT LOWER MULTIPLE  
C** SCATTERING ENERGY  
32 NC=0

C** INITIALIZE ELECTRON POSITION, ANGLE, ENERGY, AND TOP LAYER OF  
C** MATERIAL  
E=E0
C** E= ENERGY AFTER A COLLISION  
EA=E  
C** EA = ENERGY AT A BOUNDARY  
C** E AND EA HAVE DIFFERING VALUES ONLY AT BOUNDARIES  
C** COST=1.0  
C** COST=\text{COSINE OF THETA}  
SINT=0.0
**SIN** = SINE OF THETA  
COSP = 1.0  
**COS** = COSINE OF PHI  
SINP = 0.0  
**SIN** = SINE OF PHI  
THETA AND PHI ARE ANGLES OF THE SPHERICAL COORDINATE SYSTEM  
**ALF** = 0.0  
**ALF** = ALPHA = SCATTERING ANGLE WRT DIRECTION BEFORE COLLISION  
**WRT** = WITH RESPECT TO  
**COS** = COSINE OF BETA  
**BETA** = SECOND SCATTERING ANGLE WRT DIRECTION BEFORE COLLISION  
**WRT** = WITH RESPECT TO  
I = IAL  
CS = CSAL  
CE = CEAL  
CX = CXAL  
I, CE, CX, AND CS ARE VALUES OF THE PARAMETER IN A SPECIFIC REGION  
IN THIS CASE THEY ARE FOR REGION 1 AND MUST BE CHANGED IF ANOTHER MATERIAL IS TO BE USED IN ANOTHER REGION  
**XI** = X  
**XI** = X POSITION DURING TRAJECTORY  
**YI** = Y  
**YI** = Y POSITION DURING TRAJECTORY  
**ZI** = Z  
**ZI** = Z POSITION DURING TRAJECTORY  
NCOL = 0  
**NCOL** = NUMBER OF COLLISIONS  
NOUT = 0  
**NOUT** = TYPE OF OUTER BOUNDARY CROSSING  
IN THIS CASE CROSSING OF THE TOP BOUNDARY ONLY IS CONSIDERED  
**NREG** = 1  
**NREG** = THE NUMBER OF THE REGION THE ELECTRON STARTS IN  
**ESTOP** = 400.  
**ESTOP** = ENERGY AT WHICH ELECTRON TRAJECTORY IS TO BE TERMINATED  
**EMS** = EM(1)  
**EMS** = INITIAL MULTIPLE SCATTERING ENERGY
CALL SINS(62)
SINS = SINGLE SCATTERING SUBROUTINE
GOTO1000
EM=0.0
EMS IS SET = 0 TO INDICATE THAT THE ROUTINE HAS BEEN THROUGH SINS
CALL MNLS(64)
MULS = MULTIPLE SCATTERING SUBROUTINE
1000 CONTINUE
CLOSE OUT DATA SETS
1 CONTINUE
NRPR=NRPR-1
STOP
SUBROUTINE SINS(*)
THIS SUBROUTINE IS ANALOGOUS TO THE SINGLE SCATTERING PROGRAM
REAL*8 S1, S2, S3
REAL*4 I, IAL, IU, LAMG
COMMON NREG, Z0, ZB3, ZB2, ZB1, ZB0, NAB, ZI, XI, SINT, CS, YI, SINP,
IE, DES, SI, CS, SIP, SIG, CD, CE, I, NTYPE, NOUT, EA, CEL, CXAL, CSAL, IAL, SIGS,
1COST, CX, ZP1, ZP2, ZP3, ZP4, EMS, ESTOP, ISDSI, ISDTI, IS9, P1, ZMS, COSB, TPI,
3NCOL, IU, CSU, CXU, CEU, EM, LAMG, NC, NP, IE,
4ZB5, ZP5, ZB6, ZP6, ZB7, ZP7, ZB8, ZP8, ZB9, ZP9, ZB10, ZP10, ZB11, ZP11,
5ZB12, ZP12, ZB13, ZP13, ZB14, ZP14
COMMON/BINDM/S1, S2, S3, RAT, RAP, RPL, IPL, ITP, MRAN
DIMENSION RPL(2500), RAT(2500), RAP(2500), EM(25)
NAB=0
SI=CS/E
C** SI = SCREENING ANGLE
SIP=1.+SI
SIG=CE/E/E/SI/SIP
C** SIG = RUTHERFORD CROSS SECTION INTEGRATED OVER ALPHA AND BETA
DES=CE*ALOG(1.166*E/I)/E
C** DES = ENERGY LOSS PER UNIT PATH LENGTH
2 RS=RPL(IPL)
RS IS RANDOM NUMBER FOR PATH LENGTH

IPL=IPL+1
IF(IPL.LE.MRAN)GOTO30

CHECK TO SEE IF ALL RANDOM NUMBERS IN THE VECTOR HAVE BEEN USED
AND GENERATE MORE IF NECESSARY
CALL GGU1(S1,MRAN,RPL)
IPL=1
WRITE(6,210) S1
210 FORMAT('0','PATH LENGTH SEED* ,D14.7)

NTYPE=0
NTYPE=0 PATH LENGTH DOES NOT EXCEED LN(0.05)
IF(RS.GT..050) GOTO8
TO FACILITATE EXECUTION PATH LENGTHS GREATER THAN APPROXIMATELY
3*LAMDA ARE NOT USED TO KEEP LN(RS) FROM BLOWING UP
NTYPE=1
NTYPE=1 PATH LENGTH DOES EXCEED LN(0.05)
BS=.05

SIGS=-ALOG(RS)
SIGS= NO. OF MEAN FREE PATHS THE ELECTRON TRAVELS BETWEEN
COLLISIONS
S=SIGS/SIG
S = LINEAR DISTANCE
Z0=ZI+S*COST
Z0 = NEW Z COORDINATE
NCOL=NCOL+1
GOTO20

CONTINUE
CALL WRIT
SUBROUTINE WRIT IS USED TO WRITE OUT THE VARIABLES E,EA,COST,
COSP,XI,YI,ZI,DES,SINT, AND NP ONTO MAGNETIC TAPE

CALL FATE(&2,&3,G4,&7)
FATE DETERMINES BOUNDARY CROSSINGS

IF(NREG.LE.14) GOTO25
THE PROGRAM IS NOT ALLOWED INTO THE MULTIPLE SCATTERING
**SUBROUTINE UNTIL THE ELECTRON IS IN REGION 15**

IF (E .LE. EMS) GOTO 24

**EMS = ENERGY AT START OF FIRST MULTIPLE SCATTERING STEP**

**SINCE EMS = 0.0 AFTER THE PROGRAM FIRST ENTERS THE MULTIPLE SCATTERING SUBROUTINE THE PROGRAM IS THUS PREVENTED FROM RE-ENTERING THE MULTIPLE SCATTERING SUBROUTINE AFTER IT HAS RETURNED FROM THE MULTIPLE SCATTERING SUBROUTINE TO THE SINGLE SCATTERING SUBROUTINE**

25 IF (E .LE. ESTOP) RETURN

RT = RAT (ITP)

**RT IS RANDOM NUMBER THAT DETERMINES THETA**

COSB = 1. - 2. * SI * RT / (SIP - RT)

CALL GEOM

**GEOM = SUBROUTINE USED TO DETERMINE THE SCATTERING ANGLE IN THE SINGLE AND MULTIPLE SCATTERING ROUTINES**

**IT DETERMINES ALPHA, THETA, AND PHI GIVEN A BETA VALUE**

GOTO 2

3 NOUT = 1

CALL WRIT

4 RETURN

**STATEMENTS STARTING WITH 24 AND DOWN TO RETURN 1 ARE TO BACK EXTRAPOLATE PARAMETERS TO CORRESPOND TO THE INITIAL MULTIPLE SCATTERING ENERGY**

24 ED = E - EMS

SP = ED / DES

**SP = PATHLENGTH BACK TO WHERE ELECTRON HAS INITIAL MULTIPLE SCATTERING ENERGY**

ZI = ZI - SP * COST

XI = XI - SP * SINT * COSP

YI = YI - SP * SINT * SINP

**XI, YI, AND ZI ARE THE COORDINATES OF THE ELECTRON AT THE POINT IT HAS ENERGY CORRESPONDING TO THE INITIAL MULTIPLE SCATTERING ENERGY**

E = EMS

EA = E

RETURN 1

END

**SUBROUTINE FATE(*, *, *, *)**
SUBROUTINE PATE DETERMINES IF AN ELECTRON CROSSES A BOUNDARY FROM ONE REGION TO ANOTHER. IF A BOUNDARY CROSSING OCCURS THIS SUBROUTINE COMPUTES THE PATH LENGTH TO THE BOUNDARY AND THE VARIABLE VALUES AT THE BOUNDARY. IT ALSO SETS THE MATERIAL DEPENDENT PARAMETERS FOR THE MATERIAL TO BE ENCOUNTERED IN THE NEXT REGION. IT ALSO COMPUTES THE REMAINDER OF THE PATH LENGTH THAT THE ELECTRON MUST TRAVEL IN THE NEXT REGION. IF NO BOUNDARY IS ENCRYPTED THEN THE ROUTINE COMPUTES THE NEW POSITION, ENERGY AND ENERGY LOSS PER UNIT PATH LENGTH. FOR EVERY GEOMETRY TO BE STUDIED A DIFFERENT SUBROUTINE PATE MUST BE USED. THIS PATE ROUTINE HAS 14 Z BOUNDARIES TO CHECK.

REAL*4 I, IAL, IU, LAMG
COMMON NREG, Z0, ZB4, ZB3, ZB2, ZB1, ZB0, NAB, ZI, XI, S, SINT, COSP, YI, SINP, 1E, DES, SI, C, SIP, SIG, CD, CE, I, NTYPE, NOUT, EA, CEAL, CXAL, CSL, IAL, SIGS, 2COST, CX, ZP1, ZP2, ZP3, ZP4, EMS, ESTOP, ISDSI, ISDTI, ISDPI, ZMS, COSB, PI, 3NCO, IU, CSU, CXU, CED, EN, LAMG, NC, NP, IE, 4ZB5, ZP5, ZB6, ZP6, ZB7, ZP7, ZB8, ZP8, ZB9, ZP9, ZB10, ZP10, ZB11, ZP11, 5ZB12, ZP12, ZB13, ZP13, ZB14, ZP14
DIMENSION EN(25)
ZPR = ABS(ZI - Z0)
IF(ZI.NE.Z0) GOTO 2000

THIS STATEMENT CHECKS TO SEE IF THE ELECTRON PATH LENGTH IS 0 AND THE ELECTRON DOES NOT ADVANCE IN THE Z DIRECTION. THIS OCCURS IF THE ELECTRON STEP ENDS EXACTLY ON A BOUNDARY.
RETURN

STATEMENTS 1 THROUGH 13 CHECK TO SEE IF ELECTRON CROSSES A BOUNDARY.

GOTO (1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14), NREG
IF(Z0.LT.ZB14) GOTO 2000
GOTO 100
1 Z1 = Z0 - ZB0
Z2 = Z0 - ZB1
M = (Z1 + Z2) / ZP1
IF(M) 110, 100, 112
2 \( Z_1 = Z_0 - Z_B1 \)
\( Z_2 = Z_0 - Z_B2 \)
\( M = \frac{(Z_1 + Z_2)}{Z_{p2}} \)
\( \text{IF}(M) 121, 100, 123 \)

3 \( Z_1 = Z_0 - Z_B2 \)
\( Z_2 = Z_0 - Z_B3 \)
\( M = \frac{(Z_1 + Z_2)}{Z_{p3}} \)
\( \text{IF}(M) 132, 100, 134 \)

4 \( Z_1 = Z_0 - Z_B3 \)
\( Z_2 = Z_0 - Z_B4 \)
\( M = \frac{(Z_1 + Z_2)}{Z_{p4}} \)
\( \text{IF}(M) 143, 100, 145 \)

5 \( Z_1 = Z_0 - Z_B4 \)
\( Z_2 = Z_0 - Z_B5 \)
\( M = \frac{(Z_1 + Z_2)}{Z_{p5}} \)
\( \text{IF}(M) 154, 100, 156 \)

6 \( Z_1 = Z_0 - Z_B5 \)
\( Z_2 = Z_0 - Z_B6 \)
\( M = \frac{(Z_1 + Z_2)}{Z_{p6}} \)
\( \text{IF}(M) 165, 100, 167 \)

7 \( Z_1 = Z_0 - Z_B6 \)
\( Z_2 = Z_0 - Z_B7 \)
\( M = \frac{(Z_1 + Z_2)}{Z_{p7}} \)
\( \text{IF}(M) 176, 100, 178 \)

C** NUMBERS ON IF STATEMENTS REFER TO WHAT BOUNDARY WAS CROSSED

C** 178 REFERS TO A CROSSING OF ZB7 FROM REGION 7 TO REGION 8

8 \( Z_1 = Z_0 - Z_B7 \)
\( Z_2 = Z_0 - Z_B8 \)
\( M = \frac{(Z_1 + Z_2)}{Z_{p8}} \)
\( \text{IF}(M) 187, 100, 189 \)

C** 187 REFERS TO A CROSSING OF ZB7 FROM REGION 8 TO REGION 7

9 \( Z_1 = Z_0 - Z_B8 \)
\( Z_2 = Z_0 - Z_B9 \)
\( M = \frac{(Z_1 + Z_2)}{Z_{p9}} \)
\( \text{IF}(M) 198, 100, 910 \)

10 \( Z_1 = Z_0 - Z_B9 \)
\( Z_2 = Z_0 - Z_B10 \)
M = (Z1 + Z2) / ZP 10
IF (M) 1109, 100, 1111

C** 1109 INDICATES A CROSSING FROM REGION 10 TO REGION 9 ********

11 Z1 = Z0 - ZB10
Z2 = Z0 - ZB11
M = (Z1 + Z2) / ZP 11
IF (M) 1110, 100, 1112

12 Z1 = Z0 - ZB11
Z2 = Z0 - ZB12
M = (Z1 + Z2) / ZP 12
IF (M) 1211, 100, 1213

13 Z1 = Z0 - ZB12
Z2 = Z0 - ZB13
M = (Z1 + Z2) / ZP 13
IF (M) 1312, 100, 1314

14 Z1 = Z0 - ZB13
Z2 = Z0 - ZB14
M = (Z1 + Z2) / ZP 14
IF (M) 1413, 100, 1415

100 ZI = Z0

C** ROUTINE GOES TO STATEMENT 100 IF NO BOUNDARY IS CROSSED ********

C** COMPUTE A NEW ENERGY, POSITION, AND ENERGY LOSS PER UNIT PATH ********

C** LENGTH IN THE REGION
X = X + S * SINT * COSP
Y = Y + S * SINT * SINP
E = EA + DES * S
EA = E
SI = CS / E
SIP = SI + 1.
SIG = CX / E / E / SI / SIP
DES = CE * ALOG(1.166 * E / I) / E
IF (ZI.LT.ZB14) CALL WRIT
IF (NTYPE.EQ.1) RETURN 1
RETURN

110 S = (ZI-ZBQ) * S / (ZI-ZO)

C** STATEMENT 110 IS FOR CROSSING THE UPPER BOUNDARY ********

C** UPDATE POSITION, ENERGY, AND ENERGY DEPENDENT PARAMETERS ********
**Bạn đã không cung cấp nội dung để tôi đọc và tạo bản ghi tự nhiên của nó.**
NREG = 12
GOTO 106

1110 S = (ZI - ZB10) * S / (ZI - ZO)
ZI = ZB10
NREG = 10
GOTO 106

1011 S = (ZB10 - ZI) * S / (ZO - ZI)
ZI = ZB10
NREG = 11
GOTO 106

1109 S = (ZI - ZB9) * S / (ZI - ZO)
ZI = ZB9
NREG = 9
GOTO 106

910 S = (ZB9 - ZI) * S / (ZO - ZI)
ZI = ZB9
NREG = 10
GOTO 106

198 S = (ZI - ZB8) * S / (ZI - ZO)
ZI = ZB8
NREG = 8
GOTO 106

189 S = (ZB8 - ZI) * S / (ZO - ZI)
ZI = ZB8
NREG = 9
GOTO 106

178 S = (ZB7 - ZI) * S / (ZO - ZI)
ZI = ZB7
NREG = 8
GOTO 106

187 S = (ZI - ZB7) * S / (ZI - ZO)
ZI = ZB7
NREG = 7
GOTO 106

167 S = (ZB6 - ZI) * S / (ZO - ZI)
ZI = ZB6
NREG = 7
121 \( S = (ZI - ZB1) \cdot S / (ZI - ZO) \)
\( ZI = ZB1 \)
\( NREG = 1 \)
GOTO 106

112 \( S = (ZB1 - ZI) \cdot S / (ZO - ZI) \)
\( ZI = ZB1 \)
\( NREG = 2 \)
GOTO 106

203 IF (EA .GT. BUS) GOTO 101
C** THE SUBROUTINE GOES TO 203 IF THE ELECTRON ENTERS REGION 15
C** IF THE PRESENT ELECTRON ENERGY IS GREATER THAN THE STARTING
C** MULTIPLE SCATTERING ENERGY THE THE ROUTINE TRANSFERS TO 106. IF
C** NOT A STARTING MULTIPLE SCATTERING ENERGY IS OBTAINED FROM THE
C** MULTIPLE SCATTERING ENERGY MATRIX THAT IS LOWER THAN THE PRESENT
C** ELECTRON ENERGY
IE = IE + 1
EMS = EM(IE)
GOTO 203

106 CONTINUE
C** NUMBERS 10X ARE CONTINUATION STATEMENTS FOR THE XTH REGION
C** IF DIFFERENT MATERIALS ARE TO BE USED IN SEPERATE REGIONS THEN
C** INSERT MATERIAL DEPENDENT PARAMETERS AFTER PROPER CONTINUATION
C** STATEMENT
102 CONTINUE
C** AFTER 102 INSERT PROPER MATERIAL PARAMETERS FOR REGION 2
C** FOR THIS PARTICULAR CASE ONLY ONE MATERIAL IS BEING USED
C**
C** COMPUTE ENERGY AND X Y POSITION ON BOUNDARY
101 EA = EA + S * DES
\( XI = XI + S \cdot SINT \cdot COSP \)
\( YI = YI + S \cdot SINT \cdot SINP \)
CE = CEAL
CX = CXAL
CS = CSAL
I = IAL

200 SIGS = SIGS - SIG * S
C** PURPOSELY USE E RATHER THAN EA IN THE FOLLOWING SO THAT IF THE
SAME MATERIAL IS IN BOTH REGIONS, THE FINAL POSITION WILL BE IDENTICAL TO THAT IF THE BOUNDARY WAS NOT PRESENT

\[ S = \text{SIGS} / \text{SIG} \]

\[ \text{NAB} = \text{NAB} + 1 \]

\[ Z_0 = Z_1 + S \times \text{CO ST} \]

RETURN

END

SUBROUTINE NULS(*)

THIS SUBROUTINE CALCULATES MULTIPLE SCATTERING COLLISIONS USING THE PREVIOUSLY CALCULATED ENERGY, PATH LENGTH, AND CROSS SECTION INFORMATION

REAL*4 I, IAL, IU, LANG
REAL*8 S1, S2, S3, EE

COMMON NRREG, Z0, ZB4, ZB3, ZB2, ZB1, ZB0, NAB, Z1, XI, S, SINT, CS, SP, YI, SINP, I, DES, SI, CS, SIP, SIG, CD, CE, I, NTYPE, MOUT, EA, CEAL, CXAL, CSL, IAL, SIGS, 2COST, CX, ZP1, ZP2, ZP3, ZP4, EMS, ESTOP, ISDS1, ISMD1, ISDPI, ZMS, COSB, TPI, 3NCOL, IU, CSU, CXU, CEU, EM, LANG, WC, WP, IE,
4ZB5, ZP5, ZB6, ZP6, ZB7, ZP7, ZB8, ZP8, ZB9, ZP9, ZB10, ZP10, ZB11, ZP11
5ZB12, ZP12, ZB13, ZP13, ZB14, ZP14
COMMON/CMS/AMS, DELS, DE, TLEF, ID
COMMON/FM/ZA, YI, XJ
COMMON/RNDM/S1, S2, S3, RAT, RAP, RPL, IPL, ITP, MRAN
DIMENSION RPL(2500), RAP(2500), IPL(2500)
DIMENSION EE(25), EM(25), DELS(25), DE(25), AMS(25, 91), A(91),
TS(9), TLEF(25)

K = IE

IE IS THE SUBSCRIPT USED IN THE MATRIX OF MULTIPLE SCATTERING ENERGIES INDICATING AT WHAT ENERGY MULTIPLE SCATTERING SHOULD BEGIN

ZLEF = 0.

RS = RPL(IPL)
RS = PORTION OF STEP LENGTH ELECTRON TRAVELS BEFORE UNDERGOING A
COLLISION
THIS BRINGS A RANDOMNESS INTO THE LENGTH THE ELECTRONS TRAVEL
BETWEEN COLLISIONS

IPL = IPL + 1
IF (IPL .LE. MRAN) GOTO 30
CALL GGU1(S1, MRAN, RPL)
IPL = 1

30 DEX = DELS(K) * RS
DEX = PATH LENGTH TRAVELED BEFORE COLLISIONS
DET = DELS(K) - DEX
DET = PATH LENGTH TRAVELED AFTER COLLISIONS
S = DEX
Z0 = Z1 + S * COST
Z0 = NEW DISTANCE OF TRAVEL IN Z DIRECTION
GOTO 20

11 CONTINUE
CALL WRIT

WRITE = SUBROUTINE TO RECORD PARAMETERS ON TAPE

20 CALL FTEM(&10, &11, J, K)

RT = RAT(ITP)
RT = RANDOM NUMBER USED TO DETERMINE BETA
N = 90. * RT
N = N + 1
B = AMS(K, N)
C = AMS(K, N + 1) - B
D = N
G = D / 90.
P = (D + 1.) / 90.
DELTA = (RT - G) / (P - G)
N, N + 1, B, C, D, G, P, AND DELTA ARE PARAMETERS USED IN A TWO POINT
INTERPOLATION ROUTINE USED TO DETERMINE BETA
BETA = B + DELTA * C
COSB = COS(BETA)
CALL GEOM

GEOM = SUBROUTINE THAT DETERMINES ALPHA, THETA, AND PHI GIVEN A
C** VALUE OF BETA
NCOL=NCOL+1
C** NOW ALLOW THE ELECTRON TO TRAVEL THE REMAINDER OF THE MULTIPLE
SCATTERING STEP LENGTH
S=DET
Z0=ZI+S*COST
GOTO21
12 CONTINUE
CALL WRIT
21 CALL FTEM(510,512,J,K)
C** AGAIN CHECK FATE OF ELECTRON
K=K+1
E=EM(K)
C** SET E = ENERGY AT END OF STEP
EA=E
IF (K.EQ.25) RETURN
C** IF ALL MS STEPS ARE USED UP STOP TRAJECTORY
ZLEF=TLEF(K-1)
IF (ZI.GT.ZLEF) RETURN
C** IF PERPENDICULAR DISTANCE TO THE SURFACE OF THE SPECIMEN IS
C** GREATER THAN THE REMAINDER OF THE REMAINING PATH LENGTH END THE
C** TRAJECTORY
GOTO1
10 RETURN 1
C** RETURN 1 MEANS THAT THE ELECTRON IS NOW IN THE SINGLE SCATTERING
C** REGION AND THAT THE MAIN PROGRAM WILL NOW CALL THE SINGLE
C** SCATTERING ROUTINE
END
SUBROUTINE GI50M
C** THIS SUBROUTINE COMPUTES ALPHA BY GENERATING A RANDOM NUMBER AND
C** THEN MULTIPLIES IT BY 2*PI. IT THEN COMPUTES THETA AND PHI
C** UTILIZING THE GEOMETRIC RELATIONS BETWEEN COORDINATE SYSTEMS
REAL*4 I,IAL,IU,LAMG
REAL*8S1,S2,S3
COMMON NREG,Z0,ZB4,ZB3,ZB2,ZB1,ZB0,WAB,ZI,XI,S,MINT,COSP,YI,SINP,
1E,DES,SI,CS,SIP,SIG,CD,CE,I,NTYPE,NOUT,EA,CEAL,CXAL,CSAL,IAL,SIGS,
2COST,CX,ZP1,ZP2,ZP3,ZP4,EMS,ESTOP,ISDSI,ISDTI,ISDPI,ZMS,COSB,TP1,
DIMENSION BPL(2500) ,BAT(2500) ,BAP(2500)
BP=RAP(ITP)  
**BP IS THE RANDOM NUMBER THAT DETERMINES PHI********
ITP=ITP+1
IF (ITP.LE.MRAN) GOTO30
**CHECK TO SEE IF ALL RANDOM NUMBERS IN THE VECTOR HAVE BEEN USED********
**AND GENERATE MORE IF NECESSARY********
CALL GGUI(S2,MRAN,BAT)
CALL GGUI(S3,MRAN,RAP)
ITP=1
WRITE(6,200) S2,S3
200 FORMAT('THETA AND PHI SEEDS',2D14.7)
**STATEMENTS 30-71 COMPUTE NEW SCATTERING ANGLES********
30 SINB=SQRT(1.-COSB*COSB)
ALF=TPI*BP
SINA=SIN(ALF)
COSA=COS(ALF)
XMU=COST*COSB+SINT*SINB*COSA
THU=SQRT(1.-XMU*XMU)
IF (SINT.EQ.0.00) GOTO70
YYI=(COSB-COST*XMU)/SINT/THU
XXX=-SINB*SINA/THU
**XMU,THU,XXX, AND YYY ARE INTERMEDIATE VARIABLES********
PHI= YYYY*COSP-XXX*SINP
SINP= XXX*COSP+YYYY*SINP
COSP= PHI
GO TO 71
70 COSP=COSA
SINP=SINA
71 COST=XMU
SINT=THU
RETURN
END
SUBROUTINE FTEM(*,*,J,K)
REAL*4 I,IAL,IU,LAMG
COMMON NREG,Z0,ZB4,ZB3,ZB2,ZB1,ZB0,NAB,ZI, XI,S,SINT, COSP, YI, SINP,
1E, DES, SI, CS, SIP, SIG, CD, CE, I, NTYPE, NOUT, EA, CEAL, CXL, CSAL, IAL, SIGS,
2COST, CX, ZP1, ZP2, ZP3, ZP4, EMS, ESTOP, ISDSI, ISDTI, ISDPI, ZMS, COSB, TPI,
3NCOL, IU, CSU, CXU, CEU, EM, LAMG, NC, NP, IE,
4ZB5, ZP5, ZB6, ZP6, ZB7, ZP7, ZB8, ZP8, ZB9, ZP9, ZB10, ZP10, ZB11, ZP11,
5ZB12, ZP12, ZB13, ZP13, ZB14, ZP14,
COMMON/FM/ZJ, YJ, XJ
COMMON/CHS/ AMS, DELS, DE, TLEF, ID
DIMENSION EE(25), EM( 25), DELS( 25), DE( 25), AMS( 25,91), A(91),
1TS( 9), TLEF( 25), IS(4)
C** SUBROUTINE FTEM DETERMINES IF AN ELECTRON CROSSES BACK INTO THE
C** VOID CONTAINING REGION. IF THIS BOUNDARY CROSSING OCCURS THIS
C** SUBROUTINE COMPUTES THE PATH LENGTH TO THE BOUNDARY AND THE
C** VARIABLE VALUES AT THE BOUNDARY
IF (COST.GE.0.0) GOTO100
IF (Z0.LE.ZB14) GOTO123
100 ZI=Z0
C** ROUTINE GOES TO STATEMENT 100 IF NO BOUNDARY IS CROSSED
C** THIS COMPUTES A NEW ENERGY, POSITION, AND ENERGY LOSS PER UNIT
C** PATH LENGTH IN THE REGION
XI=XI+S*SINT*COSP
YI=YI+S*SINT*SINP
E=EA+S*DE( K)
EA=E
RETURN
123 SP=(ZI-ZB14) *S/(ZI-Z0)
C** THESE STATEMENTS COMPUTE THE ELECTRON ENERGY AND POSITION AT
C** BOUNDARY ZB14
ZI=ZB14
NREG=14
S=S-SP
XI=XI+SP*SINT*COSP
YI=YI+SP*SINT*SINP
Z0=ZI+S*COST
EA = EA + SP * DE(K)
CALL WRIT
RETURN1
C** RETURN 1 TELLS THE PROGRAM TO RETURN TO THE SINGLE SCATTERING PROGRAM
END
SUBROUTINE WRIT
C** SUBROUTINE WRIT RECORDS THE PARAMETERS TO BE WRITTEN ON TAPE IN A MATRIX. THE MATRIX HOLDS 250 OF THESE RECORDS WHICH IS LARGE ENOUGH FOR THIS ANALYSIS. IF ANOTHER ANALYSIS IS TO BE DONE THEN A NEW MATRIX SIZE MUST BE DETERMINED TO HOLD THE NECESSARY HISTORIES (NOTE THAT A SAFETY VALVE IS PROVIDED AND THE PROGRAM IS PROVIDED WITH A DUMP OF THE HISTORY WHEN THE CAPACITY OF THE MATRIX IS EXCEEDED.)
REAL*4 I, IAL, IU, LAMG
COMMON NREG, ZB4, ZB3, ZB2, ZB1, ZB0, NAB, ZI, XI, S, SINT, COSP, YI, SINP,
1 E, DES, SI, CS, SIP, SIG, CD, CE, I, NTYPE, NOUT, EA, CEAL, CXAL, CSAL, IAL, SIGS,
2 COST, CX, ZP1, ZP2, ZP3, ZP4, EMS, ESTOP, ISDSI, ISDTI, ISDPI, ZMS, COSB, TPI,
3 NCOL, IU, CSU, CXU, CEU, EN, LAMG, NC, NP, IE,
4 ZB5, ZP5, ZB6, ZP6, ZB7, ZP7, ZB8, ZP8, ZB9, ZP9, ZB10, ZP10, ZB11, ZP11,
5 ZB12, ZP12, ZB13, ZP13, ZB14, ZP14
COMMON/WRSP/HRT, NPW, NRPR
DIMENSION WRT(9, 250), NPW(160)
DIMENSION EM(25)
NC=NC+1
WRT(1,NC)=E
C** E= ENERGY OF ELECTRON AFTER LAST COLLISION
WRT(2,NC)=EA
C** EA= ENERGY OF ELECTRON AT THE BOUNDARY
WRT(3,NC)=COST
C** COST= COSINE OF THETA
WRT(4,NC)=COSP
C** COSP= COSINE OF PHI
WRT(5,NC)=XI
C** XI=X POSITION OF ELECTRON
WRT(6,NC)=YI
C**  YI=Y POSITION OF ELECTRON
    WRT(7,NC)=ZI
C**  ZI=Z POSITION OF ELECTRON
    WRT(8,NC)=DES
C**  DES=ENERGY LOSS PER UNIT PATH LENGTH IN EV PER ANGSTROM
    WRT(9,NC)=SINP
C**  SINP=SINE OF PHI
IF (NOUT.EQ.1)GOTO20
IF (NC.GE.250)GOTO30
RETURN
20  DO21III=1,NC
21  WRITE(13) (WRT(J,III),J=1,9),NP
WRITE(6,200) (WRT(J,NC),J=1,9),NP
C**  WHEN THE ELECTRON CROSSES THE UPPER BOUNDARY THE CONTENTS OF THE
C**  MATRIX ARE PUT ONTO TAPE
1  RETURN
30  DO31KIK=1,NC
31  WRITE(6,200) (WRT(J,KIK),J=1,9),NP
NC=0
RETURN
200 FORMAT(' ',2E12.5,2F7.3,3E12.5,2F7.3,I5)
END
Secondary Electron Production Programs

The first program calculates the secondary electron production due to incident electrons and records the number of secondary electrons produced. The program uses the recorded histories produced by the single scattering Monte Carlo program for a thin specimen of thickness equal to five times the mean free path of the secondary electrons. The user must provide the secondary electron mean free path and excitation energy. A logic diagram and program listing are given on the following pages.

A second program calculates the secondary electron production of the backscattered electron histories produced by the combined theory Monte Carlo program. The user must provide the secondary electron mean free path and excitation energy and the recorded backscattered electron histories. The program searches a history until it locates the point in the history where the electron is headed towards the specimen surface and is within five secondary electron mean free paths of the surface. The program computes the secondary production for each history. This value is recorded on magnetic tape. The secondary electron production of all histories is also calculated and recorded. A logic diagram and program listing of this program are given on the following pages.
Start

Enter secondary electron mean free path and excitation energy

Calculate maximum depth of secondary electron production

Read electron position, and cosine of the polar scattering angle from a magnetic tape storage of an electron history in a thin film

Calculate secondary electron yield for the first step of the history

Add this step's contribution to the secondary yield of this history

Read next set of electron parameters from the electron history tape

Is this a new history?

Yes

1

No

Is the electron Z coordinate greater than the maximum depth of secondary electron production?

Yes

2

No

1

Figure A4. Logic diagram for secondary electron production by primary electrons program
Calculate the secondary electron yield for this step

Set \( Z \) equal to the maximum depth of secondary electron production

Calculate the secondary electron yield of the final step of secondary electron production

Add this contribution to the total secondary electron production of this history

Add the history's contribution to the total secondary electron yield of all the histories

Has the electron data for a new history been read from the tape?

Yes

No

Read the next set of electron parameters from the magnetic tape

Figure A4 (Continued)
Write secondary electron production for all electron histories
Stop

Figure A4 (Continued)
SECONDARY ELECTRONS PRODUCED BY PRIMARY ELECTRONS

DIMENSION P(9), PP(9)
DEL=0.0
DEL=0.0
SEE=80.

SEE = SECONDARY ELECTRON EXCITATION ENERGY
BLAM=20.
BLAM = SECONDARY ELECTRON MEAN FREE PATH
READ(9, END=100) P, NP

READ ELECTRON DATA FROM THE TAPE

Z = P(7)
Z = PERPENDICULAR DISTANCE FROM THE SURFACE OF THE SPECIMEN AT THE START OF EACH STEP
COST=P(3)
COST = COS INH(THETA)
DES=P(8)

DES = ENERGY LOSS PER UNIT PATH LENGTH
DL=0.5*DES*BLAM*(1.-EXP(-Z/BLAM))/COST/SEE

DL = NUMBER OF SECONDARY ELECTRONS PRODUCED BY THE PRIMARY ELECTRON ON THE PATH BETWEEN THE SURFACE AND Z
IF(DL.GE.0.0) GOTO5

DL MUST ALWAYS BE POSITIVE
DL=-DL

DL=DEL+DL
DEL = TOTAL NUMBER OF SECONDARY ELECTRONS PRODUCED BY A PRIMARY ELECTRON

READ(9, END=100) P, NP
IF(NP.NE.NPP) GOTO20
ZP=P(7)

ZP = PERPENDICULAR DISTANCE FROM SURFACE OF THE SPECIMEN AT END OF EACH STEP
IF(ZP.LT.100.) GOTO6
ZP=100.
6 DES=P(8)
   COST=P(3)
4 DL=0.5*DES*RLAM*(EXP(-Z/RLAM)-EXP(-ZP/BLAM))/COST/SEE
   ** DL = NUMBER OF SECONDARY ELECTRONS PRODUCED BY THIS STEP **
   IF(DL.GE.0.0)GOTO2
   DL=-DL
   ** DEL = DEL + DL **
2 ZP=ZP + DEL
   ** END POSITION OF LAST STEP = START POSITION OF NEXT STEP **
   IF(ZP.GT.99.9)GOTO20
   GOTO3
20 DELT=DELT+DEL
   ** DELT = TOTAL SECONDARY ELECTRON PRODUCTION FOR THE HISTORIES **
   ** CONSIDERED **
   ** GO TO 20 IF A NEW HISTORY IS FOUND ON TAPE AND TERMINATE CALCULATION **
   ** FOR THIS HISTORY **
   DEL=0.0
   GOTO7
8 READ(9,END=100)P,NPP
7 IF(NP.EQ.NPP)GOTO8
   NP=NPP
   GOTO1
100 REWIND 9
   DELT=DELT+DEL
   WRITE(6,221)NP,DELT
   WRITE(6,222)DELT
221 FORMAT('0','PARTICLE',I5,2X,'SECONDARY YIELD',E12.5)
222 FORMAT('0','TOTAL SECONDARY YIELD',E12.5)
STOP
END
Figure A5. Logic diagram of secondary electrons produced by backscattered electrons program
Read next entry from backscattered electron history

Obtain the energy loss per unit path length, cosine of the polar scattering angle, and the next electron Z coordinate from the last entry on the tape

Has the electron emerged from the specimen?

Yes

3

No

Is the electron in the secondary production region?

No

Retain Z coordinate

4

Yes

Calculate secondary electron yield for this step

Add this step's contribution to the secondary electron production of this electron history

Retain last Z coordinate to be used in the next step

4
Figure A5 (Continued)
**SECONDARY ELECTRONS PRODUCED BY BACKSCATTERED ELECTRONS**

**DIMENSION P(9), PP(9), BP(4)**

**IP=1**

**IP= ELECTRON COUNTER**

**DELT=0.0**

**DEL=0.0**

**SY=0.025**

**SY= NUMBER OF SECONDARY ELECTRONS PRODUCED BY AN ELECTRON THAT BACKSCATTERS FROM THE SURFACE OF THE SPECIMEN WITHOUT ENTERING THE SPECIMEN**

**SEE=80.**

**SEE = SECONDARY ELECTRON EXCITATION ENERGY**

**BLAH=20.**

**BLAH = SECONDARY ELECTRON MEAN FREE PATH**

**ZBL=5.0*RLAM+50.**

**ZBL = THE DEPTH AT WHICH ELECTRONS HAVE A FINITE PROBABILITY OF REACHING THE SURFACE**

**1 READ(9,END=100)P,NP**

**READ ELECTRON DATA FROM THE TAPE**

**IF (P(7).LT.0.001)GOTO10**

**THIS IS THE CASE IF THE ELECTRON BACKSCATTERS ON THE SURFACE OF THE SPECIMEN**

**IF (P(3).GE.0.0)GOTO1**

**GET TO POINT IN THE HISTORY WHERE ELECTRON IS TRAVELING TOWARDS THE SURFACE BY FINDING THE VALUE OF THETA BETWEEN PI/2 AND PI THIS IS WHEN COSINE(THETA) IS LESS THAN ZERO**

**GOTO7**

**2 READ(9)P,NPP**

**7 IF(P(7).GT.ZBL )GOTO2**

**START PRODUCTION WHEN TRAJECTORY IS AT APPROXIMATELY THE MAXIMUM DEPTH OF SECONDARY ELECTRON PRODUCTION**

**Z=P(7)**

**Z = PERPENDICULAR DISTANCE FROM THE SURFACE OF THE SPECIMEN AT THE**
**START OF EACH STEP**

3 READ(9) PP, ZP
   ZP=PP(7)

C** ZP = PERPENDICULAR DISTANCE FROM SURFACE OF THE SPECIMEN AT END OF EACH STEP

4 DES=PP(8)
   C** DES = ENERGY LOSS PER UNIT PATH LENGTH

C0ST=PP(3)
   C** COST = COSINE(THETA)

C** IF (ZP.LT.0.001) GOTO5
   IF (ZP.LE.ZBL) GOTO4
   Z=ZP
   GOTO3

C** IF TRANSFER TO 3 INDICATES THAT THE ELECTRON IS NOW HEADED BACK INTO THE SPECIMEN

4 DL=0.50*DES*RLAM*(EXP(-ZP/RLAM)-EXP(-Z/RLAM))/COST/SEE
   C** DL = NUMBER OF SECONDARY ELECTRONS PRODUCED BY THIS STEP
   IF (DL.GE.0.0) GOTO9
   DL=-DL

C** DL MUST ALWAYS BE POSITIVE

9 DEL=DEL+DL
   C** DEL = TOTAL NUMBER OF SECONDARY ELECTRONS PRODUCED BY A PRIMARY ELECTRON
   Z=ZP

C** END POSITION OF LAST STEP = START POSITION OF NEXT STEP
   GOTO3

5 DL=0.50*DES*RLAM*(1.0-EXP(-Z/RLAM))/COST/SEE
   C** DL = NUMBER OF SECONDARY ELECTRONS PRODUCED ON FINAL STEP OUT OF THE SPECIMEN
   GOTO11

10 DL=SY
   C** PROGRAM ENDS HERE IF ELECTRON BACKSCATTERS ON THE SURFACE OF THE SAMPLE

C** GO TO 11 IF NEW HISTORY IS FOUND ON TAPE AND TERMINATE CALCULATION FOR THIS HISTORY
WRITE(10) PP(2), PP(5), PP(6), DEL, NP

** WRITE POSITION OF EMERGENCE AND ASSOCIATED SECONDARY ELECTRON YIELD ******

FOR EACH BACKSCATTERED ELECTRON ******

DELT = DELT + DEL ******

DEL = TOTAL SECONDARY ELECTRON PRODUCTION FOR THE HISTORIES ******

CONSIDERED ******

IP = IP + 1
DELT = 0.0
GOTO 1

100 REWUND 9
WRITE(6, 222) DELT, IP

221 FORMAT ('0', 'PARTICLE', I5, 2X, 'SECONDARY YIELD', E12.5, 2X, I5)
222 FORMAT ('0', 'TOTAL SECONDARY YIELD', E12.5, 'NUMBER OF PARTICLES', I5)
224 FORMAT ('0', 'E12.5', I5)
STOP
END
Subsurface Void Analysis Program

This program computes the backscattering and secondary electron yield for a specimen containing a rectangular parallelepiped void. The program uses the tape of the backscattered electron histories produced by the combined theory Monte Carlo program and the tape of the secondary electron production of these backscattered electrons. The user must supply the random number seeds and the coordinates of the rectangular parallelepiped void. The void depth must be equal to a previously recorded boundary in the tape of backscattered histories. The sum of the void depth and void thickness must also meet this requirement. The void is assumed to be symmetric with respect to the incident electron beam.

Since the only change in the electron trajectory due to the passage of the electron through the void is a change in the electron coordinates it is possible to calculate the change in X, Y, and Z coordinates due to the passage through the void. By summing the change in coordinates that occur when the electron passes through the void and adding this to the position where the electron backscattered from the solid specimen it is possible to obtain the electron position in the specimen after it has passed through the void.

For each backscattered electron history the program
locates the boundary at the top of the void when the electron is headed into the specimen and checks to see if the electron enters the top or sides of the void. It computes the change in coordinates if the electron enters the void. The program next locates the point in the history where the electron is headed towards the surface of the specimen. It adds the change in the Z coordinate to the present value of the Z coordinate and checks to see if the electron crosses the boundaries at the bottom or sides of the void. When the electron crosses a boundary the X and Y coordinates are calculated at the boundary and the program checks to see if the electron enters the void. If it does the change in coordinates is calculated. The program then finds the backscattering position of the electron on the tape and adds the sum of the change in coordinates to this position. If the new electron position is inside the specimen a single scattering Monte Carlo program is used to continue the trajectory. The trajectory is recorded above the maximum secondary electron production depth. After all backscattered electron histories are analyzed the secondary production of the new histories is computed. The program prints the new number of backscattered and secondary electrons.
Start

Initialize counting parameters

Read random number seeds

Form random number vectors

Initialize parameters for the single scattering Monte Carlo calculations

Enter secondary electron mean free path and excitation energy

Read void coordinates

Read set of electron parameters from recorded backscattered electron history on magnetic tape

Have all backscattered electron histories been read?

No

Does electron backscatter off of specimen surface?

Yes

Update counter

No

Retain electron ID number of history unchanged by the void

Figure A6. Logic diagram of the subsurface void analysis program
Figure A6 (Continued)
Does the electron enter the side of the void?

Yes

Is the electron headed towards the surface of the specimen?

Yes

Add previously calculated change of Z position due to passage through the void to the present Z position

Does the electron cross the boundary corresponding to the bottom of the void?

Yes

No

Retain previous electron parameters

Read next set of electron parameters from history tape

No

Figure A6 (Continued)
Add previously calculated change of Z position due to passage through the void to the present Z position

Does the electron cross the boundary corresponding to the bottom of the void?

Yes

Calculate the X and Y position of the electron at the bottom boundary of the void

Does the electron enter the void?

Yes

Calculate the possible path lengths the electron can travel before hitting the void wall

Choose the minimum pathlength

Calculate the corresponding change in coordinates

Sum up the total change in coordinates due to the electrons passage through the void

Read the electron parameters from the backscattered electron history tape

Figure A6 (Continued)
Read the electron parameters from the backscattered electron history tape

Calculate Z position of the electron

Is the electron above the top of the void?

Yes

No

Calculate the X and Y position of the recorded history

Does the electron enter the side of the void?

Yes

Calculate the possible path lengths the electron can travel before hitting the void wall

Choose the minimum path length

Calculate the corresponding change in coordinates

No

Figure A6 (Continued)
Add the calculated change in coordinates to the final entry of this backscattered electron history.

Is the electron now positioned below the surface of the specimen?

Yes

Start single scattering Monte Carlo calculations

Calculate the distance the electron travels on this step

Calculate the corresponding Z coordinate

Does the electron backscatter?

Yes

No

Calculate the new X and Y position, energy, mean free path, and energy loss per unit path length of the electron

Figure A6 (Continued)
Is the electron in the secondary electron production region?

Yes

Write electron parameters on an output device (tape or disk)

Calculate the scattering angles $\beta$ and $\alpha$

Calculate the scattering angles $\theta$ and $\phi$ which correspond to $\beta$ and $\alpha$

Is the electron energy less than 400 eV?

No

Is the electron Z position deeper than 4000 Å?

No

Update absorbed electron counter

Yes

Figure A6 (Continued)
250

9

Compute the electron parameters at the surface of the specimen

Write these electron parameters on an output device

11

12

Write old and new number of backscattered electrons

Read secondary electron yields of electrons whose histories are not changed when they go through a specimen containing a void

Sum this yield of secondary electrons

Read electron history produced by the single scattering Monte Carlo calculations in this program

Is the electron on the specimen surface?

Yes

13

No

6

Figure A6 (Continued)
Read next set of electron parameters from the recorded history

Is this the end of the recorded histories?

Yes → 16

No → Is the electron on the specimen surface?

Yes → 13

No → Calculate the secondary production of this step in the history

Add this to the secondary electron production of this history

Retain the previous Z position

15

Figure A6 (Continued)
Calculate the secondary electron production in the step when the electron exits the specimen surface.

Add this secondary electron production to the secondary electron production of this history.

Add the secondary electron production of this history to the total secondary production of all the histories.

Write the total number of secondary electrons produced.

Stop.
VOID ANALYSIS PROGRAM

REAL*4 I, ICU
REAL*8 S1, S2, S3
COMMON P, PP, VX, VY, VZ, VXV, VYV, DX, DY, DZ, DXP, DYP, DZP, VC
DIMENSION RPL(1000), RAT(1000), RAP(1000), P(9), PP(9), NPM(2000), R(4)
NW=10

C** RANDOM NUMBERS SEEDS
READ(5, 333) S1, S2, S3
333 FORMAT (3D14.7)

C** S1, S2, AND S3 ARE DOUBLE PRECISION

C** FORM RANDOM NUMBER VECTORS
CALL GU1(S1, 1000, RPL)
CALL GU1(S2, 1000, RAT)
CALL GU1(S3, 1000, RAP)

C** INITIALIZATION FOR MONTE CARLO ROUTINE
CS=5.449

C** CS = CONSTANT FOR SCREENING ANGLE
CX=14.4*14.4

C** CX = (CHARGE OF THE ELECTRON IN EV/ANGSTROM)**4
PI=3.14159
CNA= 0.6024

C** CNA= AVOGADRO'S NUMBER * (10)**-24
TPI=2.*PI
CE=-TPI*0.6024*14.4*14.4
ZCU=29.

C** ZCU = ATOMIC NUMBER OF AN ELEMENT
RHOCU= 8.96

C** RHOCU = DENSITY OF AN ELEMENT
ACU= 63.546

C** ACU = ATOMIC MASS OF AN ELEMENT
ICU= 377.

C** ICU = IONIZATION CONSTANT OF AN ELEMENT
CSCU= CS*ZCU**(2.0/3.0)
\[
CXCU = 0.25 \pi CX \cdot ZCU \cdot (ZCU+1) \cdot CNA \cdot RHOCU/ACU
\]
\[
CECU = CE \cdot ZCU + RHOCU/ACU
\]
\[
I = ICU
\]
\[
CS = CSCU
\]
\[
CX = CXCU
\]
\[
CE = CECU
\]

1001 READ (5,200,END=1000) VD,VX,VY,VZ

**VD = VOID DEPTH**

**VX = 0.5* VOID WIDTH**

**VY = 0.5* VOID LENGTH**

**VZ = VOID THICKNESS**

\[VC = VZ + VD\]

**VC = Z COORDINATE OF BOTTOM OF VOID**

**VOID IS SYMMETRIC WITH RESPECT TO THE Z AXIS**

WRITE (6,203) VD,VZ,VY,VX

**INITIALIZE COUNTING PARAMETERS**

\[IIB=0\]

\[ICP=0\]

\[IM=0\]

\[IP=1\]

\[IA=1\]

\[IB=0\]

\[IC=0\]

\[ICP=0\]

\[IPP=1\]

\[IUB=0\]

\[VYV=VY\]

\[VXX=VX\]

**VXX AND VYV = INTERMEDIATE VARIABLES**

11 DX=0.

\[DY=0.\]

\[DZ=0.\]

\[DXP=0.\]

\[DYP=0.\]

\[DZP=0.\]

**SET PATH LENGTHS INSIDE OF VOID TO ZERO**

1 READ(9,END=400) P,NP
ELECTRON BACKSCATTERED AT THE SURFACE OF THE SOLID SPECIMEN

IF (P(7) .EQ. 0.0) GOTO 119
IF (P(7) .EQ. VZ) GOTO 117
P(7) = Z COORDINATE
GOTO 1

119 IIB = IIB + 1
GOTO 119

117 IIB = IIB + 1
IF (ABS(P(6)) .GE. VY) GOTO 2
P(6) = Y COORDINATE OF THE ELECTRON
CHECK TO SEE IF ELECTRON MISSES VOID IN Y DIRECTION
X = P(5)
IF (ABS(X) .GE. VX) GOTO 2
CHECK TO SEE IF ELECTRON MISSES THE VOID IN THE X DIRECTION
IF (P(5) .EQ. 0.0) GOTO 21
X = P(5)
Y = P(6)
Z = P(7)
C0S = P(3)
C0SP = P(4)
SINT = SQRT(1 - C0S**2)
SINP = P(9)
SZ = VD/C0S
S = POSSIBLE DISTANCE THE ELECTRON CAN TRAVEL IN THE VOID BEFORE HITTING THE BOTTOM OF THE VOID
IF (C0SP.GT.0.0) GOTO 3
VXV = - VX
S = (VXV - X) / SINT / C0SP
\[ SX = \text{POSSIBLE DISTANCE THE ELECTRON CAN TRAVEL IN THE VOID BEFORE HITTING THE X SIDE OF THE VOID} \]

\[ 60 \text{ IF}(\text{SINP.GT.0.0}) \text{GOTO 04} \]

\[ VYV=-VY \]

\[ 4 \text{ SY}=(VYV-Y)/(\text{SINT}/\text{SINP}) \]

\[ SY = \text{POSSIBLE DISTANCE THE ELECTRON CAN TRAVEL IN THE VOID BEFORE HITTING THE Y SIDE OF THE VOID} \]

\[ S=\text{MIN1}(SX,SY,SZ) \]

\[ S = \text{MINIMUM OF SX,SY, AND SZ} \]

\[ S = \text{DISTANCE THE ELECTRON TRAVELS WITHIN THE VOID} \]

\[ DZ=S*\text{COST} \]

\[ DY=S*\text{SINT*SINP} \]

\[ DX=S*\text{SINT*COSP} \]

\[ DX, DY, \text{ AND DZ = CHANGES IN X, Y, AND Z DIRECTION OF TRAJECTORY DUE TO PASSAGE THROUGH THE VOID} \]

\[ VYV=VY \]

\[ VXV=VX \]

\[ \text{GOTO 34} \]

\[ \text{C**} \]

\[ \text{GO TO 34 IF ELECTRON HAS ENTERED THE TOP OF THE VOID} \]

\[ 21 \text{ DZ}=VD \]

\[ \text{C**} \]

\[ \text{GO TO 21 IF ELECTRON PASSES PERPENDICULARLY THROUGH THE VOID} \]

\[ \text{GOTO 34} \]

\[ \text{C**} \]

\[ \text{START CHECKING IF THE ELECTRON ENTERS THE SIDE OF THE VOID WHEN THE ELECTRON IS HEADED AWAY FROM THE SURFACE} \]

\[ 2 \text{ READ}(9, \text{END}=400)PP,NP \]

\[ \text{IF}(PP(3).LT.0.0) \text{GOTO 33} \]

\[ \text{C**} \]

\[ \text{CHECK IF THE ELECTRON IS HEADED TOWARDS THE SPECIMEN SURFACE} \]

\[ \text{IF}(PP(7).GT.VC) \text{GOTO 70} \]

\[ \text{C**} \]

\[ \text{CHECK IF THE ELECTRON IS NOW DEEPER THAN THE BOTTOM OF THE VOID} \]

\[ \text{IF}(\text{ABS}(PP(6)).GT.VY) \text{GOTO 86} \]

\[ \text{IF}(\text{ABS}(PP(5)).GT.VX) \text{GOTO 86} \]

\[ \text{C**} \]

\[ \text{CHECK IF THE ELECTRON IS INSIDE OF THE VOID} \]

\[ \text{IF}(\text{ABS}(P(6)).LE.VY) \text{GOTO 80} \]

\[ \text{IF}(\text{ABS}(P(5)).LE.VX) \text{GOTO 81} \]

\[ \text{C**} \]

\[ \text{CHECK WHETHER THE ELECTRON CROSSED THE X OR Y BOUNDARY WHEN IT ENTERED THE VOID} \]

\[ 80 \text{ NRE}=1 \]
CALL SIDE(NRE,625)
C** SUBROUTINE SIDE COMPUTES THE CHANGE IN THE ELECTRON'S POSITION
C** IF THE ELECTRON ENTERS THE SIDE OF THE VOID
81 NRE=2
CALL SIDE(NRE,625)
86 DO87J=1,9
87 P(J)=PP(J)
GOTO 2
70 IF (PP(3) .GE. 0.0) GOTO 2
GOTO 33
34 READ(9,END=400)PP,NP
IF (PP(3) .GE. 0.0) GOTO 34
C** FIND POINT IN TRAJECTORY WHERE ELECTRON IS NOW HEADED TOWARDS THE
C** SURFACE OF THE SPECIMEN
33 ZPPR=PP(7)+DZ
C** CHECK TO SEE IF THE ELECTRON REVERSES DIRECTION ON TOP OF THE VOID
IF (ZPPR.LE.VZ) GOTO 30
DO26J=1,9
26 P(J)=PP(J)
GOTO 25
22 READ(9,END=400)P,NP
25 ZPR=P(7)+DZ
IF (ZPR.LE.VC) GOTO 23
C** FIND POINT IN TRAJECTORY WHERE THE ELECTRON CROSSES THE BOTTOM OF
C** THE VOID
GOTO 22
23 COST=P(3)
S=(VC-ZPR)/COST
C** CALCULATE THE PATH LENGTH BACK TO THE BOUNDARY
SINT=SQRT(1.-COST**2)
XP=P(5)+S*SINT*P(4)+DX
YP=P(6)+S*SINT*P(9)+DY
C** CALCULATE X AND Y POSITIONS ON THE BOUNDARY AT THE BOTTOM OF THE
C** VOID
IF (ABS(YP) .GE. VY) GOTO 10
IF (ABS(XP) .GE. VX) GOTO 10
C** CHECK TO SEE IF ELECTRON MISSED VOID IN X OR Y DIRECTIONS
C** ASSIGN CORRECT VARIABLE NAMES TO POSITION AND DIRECTION PARAMETERS ******
C** X, Y, Z, COST, COSP, SINT, AND SINP HAVE THEIR PREVIOUS MEANINGS ******
C** IF THE ELECTRON ENTERS THE VOID
X = XP
Y = YP
Z = VC
COST = P(3)
COSP = P(4)
SINT = SQRT(1. - COST**2)
SINP = P(9)
C** CALCULATE DISTANCE TRAVELED IN THE VOID AND THE CHANGES IN THE X, Y, ******
C** AND Z DIRECTIONS OF THE TRAJECTORY DUE TO THE PASSAGE BACK ******
C** THROUGH THE VOID
SZ = -VD/COST
IF (COSP .GT. 0.0) GOTO 13
VXV = -VX
13 SX = (VXV - X) / SINT/COSP
61 IF (SINP .GE. 0.0) GOTO 14
VYV = -VY
14 SY = (VYV - Y) / SINT/SINP
S = AMIN1(SX, SY, SZ)
DZP = S*COST
DYP = S*SINT*SINP
DXP = S*SINT*COSP
VYV = VY
VXV = VX
GOTO 71
C** GO TO 71 IF THE ELECTRON ENTERED THE BOTTOM OF THE VOID ******
10 CONTINUE
72 READ(9, END=400) PP, NP
C** START TO CHECK IF THE ELECTRON CROSSES THE SIDE OF THE VOID WHEN ******
C** THE ELECTRON IS HEADED TOWARDS THE SURFACE
ZPR = PP(7) + DZ
YPR = PP(6) + DY
XPR = PP(5) + DX
IF (ZPR .LT. VZ) GOTO 71
C** CHECK TO SEE IF THE ELECTRON IS ABOVE THE TOP OF THE VOID ******
IF (ABS(YPR) .GT. VY) GOTO 96
IF (ABS(XPR) .GT. VX) GOTO 96
C** CHECK TO SEE IF THE ELECTRON IS INSIDE THE VOID
  YR = P(6) + DY
  XR = P(5) + DX
  IF (ABS(YR) .LE. VY) GOTO 90
  IF (ABS(XR) .LE. VX) GOTO 91
C** SEE WHETHER THE ELECTRON CROSSED THE X OR Y BOUNDARY WHEN IT
C** ENTERED THE VOID
90   NRE = 1
     CALL SIDE(NRE, &71)
91   NRE = 2
     CALL SIDE(NRE, &71)
96   DO 97 J = 1, 9
97   P(J) = PP(J)
     IF (PP(7) .EQ. 0.0) GOTO 71
     IF END OF THE HISTORY IS FOUND GO TO 71
GOTO 72
71   DZ = DZ + DZP
     DY = DY + DYP
     DX = DX + DXP
C** CALCULATE THE TOTAL CHANGE IN THE COORDINATES DUE TO THE ELECTRON
C** PASSAGE THROUGH THE VOID
   IF (DZ .LT. 0.1) GOTO 30
C** CHECK TO SEE IF THE CHANGE IN THE Z COORDINATE IS SO SMALL THAT
C** THE ELECTRON MUST AGAIN ESCAPE FROM THE SPECIMEN WITH THE SAME
C** SECONDARY ELECTRON YIELD
   IF (PP(7) .EQ. 0.0) GOTO 20
16   READ (9, END=20) PP, NP
     IF (PP(7) .NE. 0.0) GOTO 16
C** FIND THE ELECTRON DATA AT POINT OF ESCAPE FROM THE SPECIMEN
C** SET VALUE OF THE PARAMETERS NEEDED TO START THE MONTE CARLO
C** ROUTINE
20   E = PP(1)
     EA = PP(2)
     COST = PP(3)
     COSP = PP(4)
\begin{verbatim}
SINT=SQRT(1.-C0ST**2)
XI=PP(5)+DX
YI=PP(6)+DY
ZI=PP(7)+DZ
DES=PP(8)
SINP=PP(9)
WRITE(NW) E,BA,C0ST,C0SP, XI, YI, ZI, DES, SINP, NP

212 FORMAT( ' ', 2E12.5, 2F10.5, 5E12.5, 15)

C** WRITE ELECTRON DATA AT START OF ADDITIONAL TRAJECTORY
C** THIS IS THE ELECTRON DATA AT THE POINT IN THE SPECIMEN CONTAINING
C** THE VOID WHICH CORRESPONDS TO THE ESCAPE POINT OF THE BACKSCATTERED
C** ELECTRON IN THE SOLID SPECIMEN
C** A SINGLE SCATTERING ROUTINE IS USED TO CONTINUE THE HISTORIES
C** THAT NOW TERMINATE WITHIN THE SPECIMEN
C** START SINGLE SCATTERING PART OF THE PROGRAM FOR THE HISTORIES

C** MAB=0
SI=CS/E
C** SI=SCREENING ANGLE
SIP=1.+SI
NCOL=0
SIG=CI/E/E/SI/SIP
C** SIG= RUTHERFORD CROSS SECTION INTEGRATED OVER ALPHA AND BETA

102 BS=BPL(IP)
IP=IP+1
IF(IP.LE.1000) GOTO103
CALL GGU1(S1,1000,RPL)
IP=1

103 NTYPE=0.0
C** NTYPE=0 PATH LENGTH DOES NOT EXCEED LN(0.05)
IF (BS.GT.0.05) GOTO8
NTYPE=1
C** NTYPE=1 PATH LENGTH DOES EXCEED LN(0.05)
BS=0.05

8 SIGS= -ALOG (RS)
C** SIGS= NO. OF MEAN FREE PATHS THE ELECTRON TRAVELS BETWEEN
C** COLLISIONS
S=SIGS/SIG
\end{verbatim}
**S** = LINEAR DISTANCE

\[ Z_0 = Z_I + S \cdot \cos \theta \]

If \( Z_0 < 0.0 \), GOTO 110

**CHECK TO SEE IF ELECTRON CROSSES TOP OF SPECIMEN**

**UPDATE POSITION AND ENERGY DEPENDENT PARAMETERS**

\[ Z_I = Z_0 \]

\[ X_I = X_I + X \cdot \sin \theta \cdot \cos \phi \]

\[ Y_I = Y_I + S \cdot \sin \theta \cdot \sin \phi \]

\[ E = E_A + \Delta E \cdot S \]

\[ E_A = E \]

\[ S_I = S \cdot \cos \theta / E \]

\[ S_I P = \frac{1. + S}{S_I P} \]

\[ S = \exp \left( \frac{1. 166 \cdot E}{I} \right) \]

If \( Z_I > 100 \), GOTO 100

**WRITE FOR SECONDARY ELECTRON PRODUCTION**

100 IF (NTYPE.EQ. 1) GOTO 102

**COMPUTE ALPHA AND BETA AND THEN MAKE CONVERSION TO THETA AND PHI OF SPHERICAL COORDINATE SYSTEM**

\[ \beta_T = E_A \cdot T \cdot \left( \frac{IA}{E} \right) \]

\[ \alpha_P = R \cdot A \cdot P \cdot (IA) \]

\[ IA = IA + 1 \]

If \( IA \leq 1000 \), GOTO 101

CALL GGU1(S, 1000, RAT)

CALL GGU1(S3, 1000, RAP)

\[ IA = 1 \]

101 \[ \cos \beta = 1. - 2. \cdot S_I \cdot S_I T / (S_I P - S_I T) \]

\[ \sin \beta = \sqrt{1 - \cos^2 \beta} \]

\[ \alpha = T \cdot P \cdot I \cdot R \]

\[ \sin \alpha = \sin (\alpha) \]

\[ \cos \alpha = \cos (\alpha) \]

\[ \chi = \cos \theta \cdot \cos \beta + \sin \phi \cdot \sin \beta \cdot \cos \alpha \]

\[ \theta = \sqrt{1 - \chi^2} \]

\[ Y_{1} = (\cos \beta \cdot \cos \chi) / \sin \theta \cdot \sin \phi \]

\[ X_{11} = -\sin \beta \cdot \cos \alpha / \sin \theta \cdot \sin \phi \]

\[ \phi = Y_{11} \cdot \cos \theta \cdot \chi \]

**WRITE FOR SECONDARY ELECTRON PRODUCTION**
SI NP=XXX*COSP+YYY*SINP
COSP=PHI
COST=XMU
SINT=TMU
NCOL=NCOL+1
IF(E.LE.400.)GOTO300
IF(ZI.GT.4000.)GOTO300
GOTO102

110 S=ZI*S/(Z0-ZI)

C** COMPUTE POSITION AND ENERGY AT POINT OF ELECTRON EMERGENCE ******

ZI=0.0
XI=XI+S*SINT*COSP
YI=YI+S*SINT*SINP
EA=EA+S*DES
IB=IB+1
WRITE(NW)E,EA,COSP,COST,KI,YI,ZI,DES,SISP,NP
GOTO11

300 IC=IC+1
C** IC = NUMBER OF TRAJECTORIES THAT PASSED THROUGH THE VOID BUT DID NOT******
C** BACKSCATTER ******
GOTO11

30 DX=0.
DY=0.
DZ=0.
DZP=0.
DYP=0.
DXP=0.
IM=IM+1
NPM(IM)=NP
ICP=ICP+1
32 READ(9,END=400)P,NPP
C** FIND NEW TRAJECTORY ON TAPE ******
IF(P(7).EQ.0.0)GOTO1
GOTO32

400 IND=IB+ICP
C** IND = NUMBER OF BACKSCATTERED ELECTRONS OF A SPECIMEN CONTAINING THE******
C** VOID ******
WRITE (6,201) IIB, INB

201 FORMAT('0', 'OLD + NEW NUMBER OF BACKSCATTER', I5, 2X, I5)
ENDFILE NW
REWIND NW
REWIND 9
DELT=0.0
READ(11,END=42) R, NPP

C** FOR ELECTRON HISTORIES THAT ARE UNCHANGED FIND SECONDARY ELECTRON
C** YIELD ON TAPE AND ADD UP TOTAL SECONDARY YIELD FROM ALL UNCHANGED
C** HISTORIES
D040 I=1,IM
NI.>=NPH(II)
G0T043
41 READ(11,END=42) R, NPP
43 IF (NP.NE.NPP) G0T041
DELT=DELT+R(4)
40 CONTINUE
42 IPP=IM

C** THIS PART OF THE PROGRAM COMPUTES THE NUMBER OF SECONDARY ELECTRONS
C** DUE TO THE NEW BACKSCATTERED ELECTRON HISTORIES
C** IT IS IDENTICAL TO THE PROGRAM THAT CALCULATES SECONDARY ELECTRON
C** PRODUCTION DUE TO BACKSCATTERED ELECTRONS
DELT=0.0
SEE=80.
RLAM=20.
51 READ(NW,END=900) P, NP
57 Z=P(7)
53 READ(NW,END=900) PP, NPP
52 ZP=PP(7)
IF(ZP.LT.0.001) G0T055
55 READ(NW,END=900) PP, NPP
56 DES=PP(8)
COST=PP(3)
IF(COST.LT.0.0) G0T054
COST=-COST
54 DL=0.50*DES*RLAM*(EXP(-ZP/RLAM)-EXP(-Z/RLAM))/COST/SEE
IF (DL .GE. 0.0) GOTO 59
DL = -DL

59 DL = DEL + DL
Z = ZP
GOTO 53

55 DL = 0.50 * DBS * RLAM * (1.0 - EXP(-Z / RLAM)) / COST / SEE
DEL = DEL + DL
DELT = DELT + DEL
IPP = IPP + 1
DEL = 0.0
GOTO 51

56 DEL = DEL + DL
DELT = DELT + DEL
IPP = IPP + 1
DEL = 0.0
WP = NPP
GOTO 57

900 REWIND NW
REWIND 11
WRITE (6, 222) DELT, IPP
GOTO 1001

222 FORMAT ('0', 'TOTAL SECONDARY YIELD', E12.5, 'NUMBER OF PARTICLES', I5)
200 FORMAT (5E12.5)
203 FORMAT ('1', 'VOID THICKNESS', F6.2, 3X, 'TOP OF VOID COOR', F6.2, 3X,
'X COOR', F6.2, 3X, 'Y COOR', F6.2)

1000 CONTINUE
STOP

END

C** SUBROUTINE SIDE COMPUTES THE CHANGE IN ELECTRON COORDINATES IF THE
C** ELECTRON ENTERS THE VOID THROUGH A SIDE OF THE VOID
C** SUBROUTINE SIDE(NRE,*)
C** COMMON P,PP,VX, VY, VZ, VXV, VYV, DX, DY, DZ, DXP, DYP, DZP, VC
C** DIMENSIONP (9), PP (9)
C** THE PP VECTOR CONTAINS THE ELECTRON DATA FOR THE ELECTRON INSIDE
C** OF THE VOID
C** THE P VECTOR CONTAINS ELECTRON DATA FOR THE ELECTRON IMMEDIATELY
C** BEFORE THE ELECTRON ENTERED THE VOID
X=PP (5)
Y=PP (6)
Z=PP (7)
COST=P (3)
COSP=P (4)
SINT=SQR (1.-COST**2)
SINP=P (9)
XP=P (5)
YP=P (6)
ZP=P (7)

IF (COST.GT.0.) GOTO 30

C** IF THE ELECTRON IS HEADED TOWARDS THE SURFACE ADD THE CHANGES IN
C** COORDINATES DUE TO THE ELECTRON PASSAGE THROUGH THE VOID ON THE
C** ELECTRON'S TRAJECTORY HEADED AWAY FROM THE SURFACE TO THE PRESENT
C** ELECTRON POSITION

X  = X + DX
XP = XP + DX
Y  = Y + DY
YP = YP + DY
Z  = Z + DZ
ZP = ZP + DZ

30 IF (NRE.GT.1) GOTO 2

C** IF THE ELECTRON CROSSED THE X BOUNDARY GO TO 2
C** IF (YP.LE.0.0) GOTO 10

DY1 = VY - Y

C** COMPUTE THE DIFFERENCE IN THE Y POSITION BETWEEN THE VOID WALL
C** AND THE ELECTRON POSITION IN THE VOID

GOTO 11

10 DY1 = Y - VY

C** COMPUTE THE DIFFERENCE IN THE Y POSITION BETWEEN THE VOID WALL
C** AND THE ELECTRON POSITION IN THE VOID

11 S = ABS (DY1/SINT/SINP)

C** COMPUTE THE CORRESPONDING PATH LENGTH

DX1 = S*SINT*COSP
DZ1 = S*COST

C** COMPUTE X AND Z CHANGES IN COORDINATES DUE TO THE ELECTRON NOW
C** BEING POSITIONED INSIDE OF THE VOID
IF (COST) 61, 61, 60
C** DETERMINE IF THE ELECTRON IS HEADED TOWARDS OR AWAY FROM THE SURFACE
C** 2 IF (XP.LE.0.0) GOTO 20
   DX1=VX-X
C** COMPUTE THE DIFFERENCE IN THE X POSITION BETWEEN THE VOID WALL AND THE ELECTRON POSITION INSIDE THE VOID
GOTO 21
C** 20 DX1=X-VX
C** COMPUTE THE DIFFERENCE IN THE X POSITION BETWEEN THE VOID WALL AND THE ELECTRON POSITION INSIDE THE VOID
C** 21 S=ABS(DX1/SINT/C0SP)
C** COMPUTE THE CORRESPONDING PATH LENGTH
   DY1=S*SINT*SINP
   DZ1=S*C0ST
C** COMPUTE Y AND Z CHANGES IN COORDINATES DUE TO THE ELECTRON NOW BEING INSIDE OF THE VOID
C** IF(COST.GT.0.0) GOTO 60
C** CHECK IF THE ELECTRON IS HEADED AWAY FROM THE SURFACE
C** 61 SZ=(VZ-Z)/COST
C** COMPUTE ELECTRON PATH LENGTH TO A Z BOUNDARY OF THE VOID
GOTO 62
C** 60 SZ=(VC-Z)/COST
C** COMPUTE ELECTRON PATH LENGTH TO A Z BOUNDARY OF THE VOID
C** 62 IF(COSP.GT.0.0) GOTO 12
   VXV=-VX
C** COMPUTE THE ELECTRON PATH LENGTH TO AN X BOUNDARY OF THE VOID
   SX=(VXV-X)/SINT/COSP
C** IF(SINP.GT.0.0) GOTO 13
   VYV=-VY
C** 12 SY=(VYV-Y)/SINT/SINP
C** COMPUTE ELECTRON PATH LENGTH TO A Y BOUNDARY OF THE VOID
C** 13 S=AMIN1(SX,SY,SZ)
C** CHOOSE THE MINIMUM PATH LENGTH
C** IF (COST.LE.0.0) GOTO 14
C** 14 DZ=DZ1+S*C0ST
C** DS=DS1+S*SINT*SINP
C** IF (COST.GT.0.0) GOTO 70
C** ASSUMING THE ELECTRON IS HEADED AWAY FROM THE SURFACE
DX = DX1 + S * SINT * COSP

**Calculate corresponding X, Y, and Z coordinate changes due to the electron traveling a path length in the void**

GOTO 15

14 DZP = DZ1 + S * COST
   DYP = DY1 + S * SINT * SINP
   DXP = DX1 + S * SINT * COSP

**Calculate corresponding X, Y, and Z coordinate changes due to the electron traveling a path length in the void**

15 VXV = VX
   VYV = VY
   IF (COST .LE. 0.0) GOTO 83
   GOTO 84

80 READ (9) P, NP
   ZPR = P (7) + DZ

84 IF (ZPR GT. VC) RETURN 1

**If the electron is headed away from the surface find point in the trajectory where the electron is below the bottom of the void**

GOTO 80

81 READ (9) P, NP
   ZPR = P (7) + DZP + DZ

83 IF (ZPR LE. VZ) RETURN 1

**If the electron is headed towards the surface find the point in the trajectory where the electron is above the top of the void**

IF (P (7) .EQ. 0.0) RETURN 1

**Or when the end of the recorded trajectory is found**

GOTO 81

END
APPENDIX B: SINGLE SCATTERING THEORY AND COMPUTER ALGORITHM FOR COMPOUNDS AND ALLOYS

The single scattering simulation for multiple element systems is similar to single scattering for a single element. Again we will use the Rutherford cross section for each element,

\[
d\sigma_j(\beta)/d\Omega = \left[ Z_j (Z_j+1) e^4 / 4E^2 \right] (1 - \cos \beta + 2\beta_s)_{s_j} \tag{B-1}
\]

where the subscript \( j \) refers to the \( j \)th element in the compound or alloy. It is assumed that the electron interacts with one atom at a time and it is necessary to determine with which elemental atom the electron interacts. The number of atoms of a given element per unit volume is \( N_j \) and is given by

\[
N_j = c_j \rho N_o / A_j \tag{B-2}
\]

where \( A_j \) and \( c_j \) are the atomic weight and weight fraction of the \( j \)th atom, respectively. \( N_o \) is Avogadro's number and \( \rho \) is the density of the compound or alloy. Denoting \( \sigma_j(E) \) as Equation B-1 integrated over all angles of scattering, the probability that the incident electron encounters anyone of the \( j \)-atoms in order to change its direction of motion is proportional to \( N_j \sigma_j(E) \). Thus when a random number, \( R_2 \), is generated in the calculational procedures that satisfies
the criterion

\[ R_2 < \frac{N_1 \sigma_1(E)}{\sum_j N_j \sigma_j(E)} \]  

one may consider that the electron is scattered by an atom of element 1. The possibility of scattering by an atom of element 2 is given by the random number, \( R_2 \), which satisfies

\[ \frac{[N_1 \sigma_1(E)/\sum_j N_j \sigma_j(E)]}{\leq R_2 < \{[N_1 \sigma_1(E)+N_2 \sigma_2(E)]/\sum_j N_j \sigma_j(E)\}} \]

and this process can be extended for any number of elements. The new direction of motion of the electron after the collision is described by Equation B-1 using the proper element in the expression.

The path length is again determined by the mean free path of the incident electrons. In this case \( \lambda \) is given by

\[ \frac{1}{\lambda} = \sum_j \frac{1}{\lambda_j} = \sum_j N_j \sigma_j(E) \]  

where the summation is carried over the different elements in the compound. The energy loss due to the inelastic collisions is taken into account by averaging the loss due to the individual elements using the extended Bethe energy loss equation. The equation is

\[ \frac{dE}{dS} = (2\pi e^4 N_0/E) \sum_j \left(C_j Z_j/A_j\right) \ln(1.166 E/I_j) \]  

(B-6)
These equations can be combined into a single scattering theory Monte Carlo method algorithm for multiple element systems. The steps of the algorithm are:

1. Initialize the energy, $E_0$, position, $r_0$, and direction of travel $\Omega_0(\theta, \phi)$, of the electron.

2. Determine the distance the electron travels before undergoing a collision with an atom:

$$\Delta S_n = -\ln(R_\perp) \sum_j N_j \sigma_j(E)$$

where $R_\perp$ is a random number.

3. Determine the electron energy at the end of the step, $E_{n+1}$.
   a. Use the Bethe energy loss equation, Equation B-6, to determine $(dE/dS)_n$.
   b. Determine $E_{n+1}$ using the equation

$$E_{n+1} = E_n - \Delta S_n (dE/dS)_n$$

4. Determine which species of atom the electron collides with according to the criteria in Equations B-3 and B-4.

5. Determine the new direction of travel.
   a. Determine the polar angle of scattering

$$\cos \beta = 1 - \left[2\beta s_j R_3/(1 + \beta s_j - R_3)\right]$$
where \( R_3 \) is a random number and \( \beta_{s_j} \) is the screening angle for the \( j_{th} \) element.

b. Determine the azimuthal angle of scattering

\[ \alpha = R_4 2\pi \]

where \( R_4 \) is a random number.

c. Compute \( \theta_{n+1} \) and \( \phi_{n+1} \) corresponding to \( \beta \) and \( \alpha \) using the geometric relationships in Equations 10, 11 and 12 of the text.

6. Check position and energy of the electron to see if the history can be terminated. If the history is not terminated return to step 2. If the history is terminated return to step 1.

The logic diagram and listing of the program using this algorithm are shown on the next pages.
Figure B1. Logic diagram of the single scattering Monte Carlo program for alloys and compounds.
1. Calculate the path length the electron travels.

2. Calculate the corresponding Z coordinate.

   a. Does the electron cross the upper specimen boundary?
      - Yes → 2
      - No → 3

3. Calculate the new electron coordinates, and electron energy.

4. Determine which element atom the electron is to collide with next.

5. Calculate the azimuthal, α, and zenithal, β, scattering angles with respect to the direction of the electron travel in the previous step.

6. Calculate the azimuthal, φ, and zenithal, θ, scattering angles with respect to the incident electron beam direction.

7. Is the electron energy less than 600 eV?
   - Yes → 4
   - No → 5

Figure B1 (Continued)
Calculate the electron parameters at the boundary and record these parameters.

Figure B1 (Continued)
SINGLE SCATTERING MONTE CARLO PROGRAM

FOR NONRELATIVISTIC INCIDENT ELECTRON ENERGIES

THIS PROGRAM IS DESIGNED FOR ALLOYS AND COMPOUNDS

REAL*8 S1, S2, S3, S4
REAL*4 I, IAL, IC, ISI, IAU
DIMENSION BRC(7), RPL(3000), RAT(3000), RAP(3000), RPE(3000)
MRAN=3000

MBAN= SIZE OF RANDOM NUMBER VECTOR
S1=.1234570 00
S2=.325017 I 00
S3=.567912430 00
S4=0.123459 D 00

S1, S2, S3, and S4 are random number generator seeds
ALL RANDOM NUMBER GENERATOR SEEDS MUST BE ODD $$$$$$

S1, S2, S3, and S4 are double precision

IPA=1
ITP=1
IPE=1

IPA, ITP, and IPE are random number counters
USED TO CHECK NUMBER OF RANDOM NUMBERS USED OUT OF VECTOR

CS=5.449

CS = constant for screening angle

CX=14.4*14.4

CX = (charge of the electron in ev/angstrom) **4

PI=.314159E 01
CN=0.6024

CNA= AVOGADRO'S NUMBER * (10)**-24

TPI=.2E 01*PI

CE=-TPI*0.6023*14.4*14.4

EIN=10000.

EIN = INCIDENT ENERGY OF ELECTRONS

X=0.
Y=0.
Z=0.

C** X,Y,Z = INCIDENT ELECTRON BEAM POSITION

NPARS=1

C** NPARS = STARTING HISTORY INDEX

NPART=1000

C** NPART = FINISHING HISTORY INDEX

C** MATERIAL DEPENDENT PARAMETERS FOLLOW

ZCU=29.

C** ZCU = ATOMIC NUMBER OF COPPER

RHOCU=8.96

C** RHOCU = DENSITY OF COPPER

ACU=63.546

C** ACU = ATOMIC WEIGHT OF COPPER

ICU=377.

C** ICU = IONIZATION CONSTANT OF COPPER

ZAU=79.

C** ZAU = ATOMIC NUMBER OF GOLD

RHOAU=19.32

C** RHOAU = DENSITY OF GOLD

AAU=197.0

C** AAU = ATOMIC WEIGHT OF GOLD

IAU=1071.

C** IAU = IONIZATION CONSTANT OF GOLD

CCU=0.8

C** CCU = WEIGHT FRACTION OF COPPER

CAU=0.2

C** CAU = WEIGHT FRACTION OF GOLD

ROCOM=CCU*RHOCU+CAU*RHOAU

C** ROCOM = AVERAGE DENSITY OF THE ALLOY

CSCU=CS*ZCU*(.2E0/.3E0)

C** CSCU = CONSTANT FOR SCREENING ANGLE FOR COPPER

CSAU=CS*ZAU*(2.0/3.0)

C** CSAU = CONSTANT FOR SCREENING ANGLE FOR GOLD

CXCUCU=0.2500*PI*CX*ZCU*(ZCU+1.)*CNA*ROCOM/ACU

C** CXCUCU = CONSTANT FOR CROSS SECTION FOR COPPER

CXAUCU=0.25*PI*CX*ZAU*(ZAU+1.)*CNA*ROCOM/AAU
C** CXAU = CONSTANT FOR CROSS SECTION FOR GOLD
CECU = ZCU * RHOCU / ACU
C** CECU = CONSTANT FOR DETERMINING ENERGY LOSS FOR COPPER
CEAU = ZAU * RHAU / AUAU
C** CEAU = CONSTANT FOR DETERMINING ENERGY LOSS FOR GOLD
WRITE (6, 63)
63 FORMAT ('1', 'ELECTRON HISTORIES FOLLOW', '//' )
NP = 0
WRITE (6, 64)
64 FORMAT ('0', 'RANDOM NUMBER SEEDS')
65 FORMAT ('0', 3D14.7)
WRITE (6, 62)
CALL GGU1 (S1, MRAN, RPL)
C** GGU1 IS A IMSL SUBROUTINE THAT GENERATES A SET OF PSEUDO RANDOM
C** NUMBERS EQUALLY DISTRIBUTED BETWEEN 0 AND 1
C** MRAN = NUMBER OF RANDOM NUMBERS IN A VECTOR
C** RPL = VECTOR OF PATH LENGTH RANDOM NUMBERS
C** S1, S2, S3, AND S4 = RANDOM NUMBER SEEDS. THE CALLING VALUE IS
C** REPLACED WITH A NEW VALUE OF THE SEED UPON RETURN FROM GGU1
C** CALL GGU1 (S2, MRAN, RAT)
C** RAT = VECTOR OF THETA ANGLE RANDOM NUMBERS
CALL GGU1 (S3, MRAN, RAP)
C** RAP = VECTOR OF PHI ANGLE RANDOM NUMBERS
CALL GGU1 (S4, MRAN, RPE)
C** RPE = VECTOR OF RANDOM NUMBERS FOR DETERMINING SCATTERING ATOM
ESTOP = 600.
C** ESTOP = MINIMUM ELECTRON ENERGY CONSIDERED
DO 1NP = NPARS, NPART
C** DO LOOP ON HISTORIES
C** INITIALIZE ELECTRON POSITION, ANGLE, ENERGY, AND MATERIAL
COST = 1.0
C** COST = COSINE OF THETA
SINT = 0.0
C** SINT = SINE OF THETA
COSP = 1.0
C** COSP = COSINE OF PHI
SINP = 0.0
**SINP** = SINE OF PHI

**ALF** = 0.0

**COSB** = COSINE OF BETA

**NEVE** = -1

**NEVE = NUMBER OF EVENTS (COLLISIONS + BOUNDARY CROSSINGS) ELECTRON UNDERGOES DURING A TRAJECTORY**

**NEV** = NUMBER OF EVENTS (COLLISIONS + BOUNDARY CROSSINGS) ELECTRON UNDERGOES DURING A TRAJECTORY

**NCOL** = 0

**NCOL = NUMBER OF COLLISIONS**

**E** = ENERGY AFTER A COLLISION

**EA** = ENERGY AT A BOUNDARY

**E AND EA HAVE DIFFERING VALUES ONLY AT BOUNDARIES**

**XI** = X POSITION DURING TRAJECTORY

**YI** = Y POSITION DURING TRAJECTORY

**ZI** = Z POSITION DURING TRAJECTORY

**PRINT RANDOM NUMBER SEEDS ON THE LAST TRAJECTORY**

IF (NP.LT.NPART) GOTO 21
WRITE(6,64)
WRITE(6,65) S1, S2, S3
21 NAB = 0
2 SIC = CSCU/B

**SIC = SCREENING ANGLE FOR COPPER**

**SIA = SCREENING ANGLE FOR GOLD**

**SIPC = 1.0 + SIC**

**SIPA = 1.0 + SIA**

**SIGC = CCU*CXCU/E/E/SIC/SIPC**
SIGC = RUTHERFORD CROSS SECTION INTEGRATED OVER ALL SCATTERING

ANGLES FOR COPPER
SIGA = CAU*CAU/E/E/SIA/SIPA

ANGLES FOR GOLD

DES = CE*(CCU*CECU*ALOG(1.156*E/ICU) + CAU*CAU*ALOG(1.166*E/IAU))/E

DES = ENERGY LOSS PER UNIT PATH LENGTH
RS = RPL(IPA)
RS IS RANDOM NUMBER FOR PATH LENGTH
IPA = IPA + 1
IF (IPA.LE.MRAN) GOTO 30

CHECK TO SEE IF ALL RANDOM NUMBERS IN THE VECTOR HAVE BEEN USED
AND GENERATE MORE IF NECESSARY
CALL GGU1(S1,MRAN,RPL)
IPA = 1

NTYPE = 0
PATH LENGTH DOES NOT EXCEED LN(0.05)
TO FACILITATE EXECUTION PATH LENGTHS GREATER THAN APPROXIMATELY
3*LAMDA ARE NOT USED TO KEEP LN(RS) FROM BLOWING UP
IF (RS.GE.0.05) GOTO 8

NTYPE = 1
PATH LENGTH DOES EXCEED LN(0.05)
RS = 0.05

SIGS = ALOG(RS)
SIGS = NO. OF MEAN FREE PATHS THE ELECTRON TRAVELS BETWEEN
COLLISIONS
SIGT = SIGC + SIGA
SIGT = SUM OF ELEMENTAL MACROSCOPIC CROSS SECTIONS
S = SIGS/SIGT

S = LINEAR DISTANCE
ZO = ZI + S*COST

ZO = NEW Z COORDINATE

NEVS = NEVS + 1
IF (Z0.LE.0.0) GOTO 4

CHECK IF ELECTRON BACKSCATTERS
UPDATE POSITION AND ENERGY
ZI = Z0
XI = XI + S * SINT * COSP
YI = YI + S * SINT * SINP
E = EA + DES * S
EA = E
IF (NTYPE.EQ.1) GOTO 2
BOUN = SIGC / SIGT
C** BOUN = PARAMETER TO DETERMINE WHICH ELEMENTAL ATOM THE ELECTRON COLLIDES WITH NEXT
REL = RPE(IPE)
IPE = IPE + 1
IF (IPE.LE.MBAN) GOTO 24
CALL GGU1(S4, MBAN, RPE)
IPE = 1
PREP = RPE(IPE)
IPE = IPE + 1
IF (IPE.LE.MRAN) GOTO 24
CALL GGU1(S4, MRAN, RPE)
IPE = 1
C** STATEMENTS 31-73 COMPUTE NEW SCATTERING ANGLES
SINB = SQRT(1. - COSB*COSB)
ALF = TPI*RP
SINA = SIN(ΑLF)
COSA = COS(ΑLF)
XMU = COST*COSB+SINT*SINB*COSA
TMU = SQRT(1. - XMU*XMU)
IF (SINT.EQ.0.00) GOTO 70
YYY = (COSB-COST*XMU)/SINT/TMU
XXX = -SINB*SINA/TMU

C**
XMU, TMU, XXX, AND YYY ARE INTERMEDIATE VARIABLES

COST = XMU
SINT = TMU
NC01 = NC01 + 1
IF (B. LT. ES 101?) GOTO 111
C**
CHECK IF ELECTRON ENERGY IS LESS THAN THE MINIMUM
GOTO 2
4 S = ZI*S/(Z0 - ZI)
C**
STATEMENT 4 IS THE TERMINATION FOR BACKSCATTERED ELECTRONS
ZI = 0.0
XI = XI + S*SINT*COSP
YI = YI + S*SINT*SINP
E = EA + DES*S
111 WRITE(6, 60) NP, E, EA, COST, COSP, XI, YI, ZI, DES, SINP
GOTO 1
60 FORMAT('0', 'I', 'S', '1', 'E12.5', '2F7.3', '3E12.5', '2F7.3')
1 CONTINUE
11 CONTINUE
STOP
END