Predicting ultrasonic grain noise in polycrystals: A Monte Carlo model

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Abstract
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Keywords
time domain analysis, ultrasonic testing, polycrystals, grain boundaries, noise, microstructure, Monte Carlo method, backscattering

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A Monte Carlo technique is described for predicting the ultrasonic noise backscattered from the microstructure of polycrystalline materials in a pulse/echo immersion inspection. Explicit results are presented for equiaxed, randomly oriented aggregates of either cubic or hexagonal crystallites. The model is then tested using measured noise signals. Average and peak noise levels and the distribution of the noise voltages are studied as the density of grains changes. © 1996 Acoustical Society of America.

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INTRODUCTION

In ultrasonic inspections for small or subtle defects in polycrystals, defect signals may be obscured by grain noise echoes that arise from the scattering of sound by grain boundaries and other microstructural inhomogeneties. Understanding these noise signals is essential to improving the detection process. For example, there exist algorithms\(^1\)\(^–\)\(^3\) that have been developed specifically to reduce the ultrasonic grain noise. These models use signal processing techniques such as split-spectrum processing, spatial averaging, and bandpass filtering to enhance the signal-to-noise ratio. Their efficacy depends on the statistics which govern the temporal and spatial distributions of grain noise signals.

It is not only desirable to understand the statistics of the noise, but how the noise is related to the microstructure. This information is important to materials scientists, who seek to minimize noise by changes in the materials processing procedures. In addition the grain noise signals also contain useful information about the microstructure of the material. For example, a number of authors have related these signals to the ultrasonic grain size.\(^4\)\(^–\)\(^6\) Again, a detailed knowledge of the statistics of grain noise signals is central to the complete development of these techniques.

A number of models have been developed which predict noise statistics and/or relate the backscattered noise to the microstructure, with various levels of detail. In addition to the models contained in the above-cited references, Margetan \textit{et al.}\(^7\)\(^–\)\(^9\) have developed an independent scattering model (ISM) which provides a prediction of the root-mean-square (rms) grain noise in terms of a product of factors describing the measurement system and material microstructure. The latter factors have been clarified by the work of Rose,\(^10\)\(^–\)\(^12\) which provides a quantitative framework for relating the backscattering coefficient, which controls the rms noise, to the microstructure. Vergara-Dominguez and Paez-Borrallo\(^13\) have also modeled the backscattering problem in polycrystals. Although the microstructure is not introduced in a fashion as explicit as in the other work cited above, they go further toward the prediction of probability densities and space-time correlation functions of the grain noise complex envelope. They introduce the notion that form factors, controlling the noise, are random variables having a \(K\)-type probability distribution function, and explore a number of implications of this assumption on the statistical characteristics of backscattered noise. In the closely related area of tissue characterization, Narayanan \textit{et al.}\(^14\) have also used the \(K\) distribution to describe non-Rayleigh distribution of backscattering, and Chen \textit{et al.}\(^15\) have further studied non-Gaussian and non-Rayleigh statistical properties. Additional citations to work in the tissue characterization field can be found in the latter references.

Average noise levels, although useful, are not sufficient for assessing flaw detection reliability or for providing a basis for fully recovering the microstructural information contained in backscattered signals. The distributional information in Ref. 13 is a step in the right direction, but lacks an explicit connection to the microstructure. Furthermore, for various situations, one would like to have simulated time domain waveforms rather than their statistical properties.

In this work, we present a Monte Carlo method (MCM)\(^16\) for simulating time-domain noise signals observed in pulse/echo immersion inspections of polycrystalline components. The method predicts simulated time-domain noise signals, and hence can be used to determine average and peak noise levels, as well as other statistical quantities. We assume that the backscattered noise is dominated by the single scattering of the incident beam by individual crystallites. The component volume is represented as an ensemble of spherical, single-crystal grains whose centers and orientations are randomly chosen. Thus, there is an explicit link between our predictions and the microstructure, a feature not contained in the previously cited work. In Sec. I, we describe in detail the model. Section II discusses applications, including the relationship to previous work. Conclusions are presented in Sec. III.

I. MODEL DEVELOPMENT

A. Strategy

The strategy for our Monte Carlo simulations is to create an ensemble of statistically equivalent microstructures and to explicitly calculate the time domain backscattered signals from each. These signals can either be used individually in various simulations, e.g., studies of the efficacy of noise sup-
expression techniques, or they can be combined to determine various statistical properties of the backscattered noise. The individual members of the ensemble are created by first randomly positioning the grain centers, and then assigning each spherical grain a diameter such that the sums of the volumes of the grains equals that volume of the region of interest. The scattering from each grain is then analyzed as if it were embedded in an effective medium whose properties are given by the Voigt approximation, a process that has been validated by comparison to the other techniques for the special case of predicting the rms noise.\(^9\) It is obvious that the above procedure is somewhat unrealistic, in that space cannot be filled by spherical grains. It is our assumption that the condition that volume be conserved provides a first order correction. More specifics of the procedure follow. Implicit in our calculation is the assumption that the ultrasound scatters only once from each grain. Rose\(^1\) notes that this assumption should be valid at early times for which attenuation is negligible and successful comparisons of the predictions of the ISM,\(^2\) which is based on the same assumption, to experiment support this assertion. Han and Thompson\(^17\) present some heuristic arguments suggesting the conditions under which this assumption is valid.

### B. Generation of grains and signals

We consider the normal-incidence inspection geometry of Fig. 1, in which a flat polycrystalline specimen is inspected in the pulse/echo mode. We assume that a front-surface “reference” echo from the specimen has been measured when the waterpath is \(z_{0R}\). This echo serves to identify the spatial content of the incident sound beam, and the efficiency of the transducer for converting electrical energy to sound and vice versa. For a spherically focused transducer, the reference waterpath \(z_{0R}\) is set equal to the geometrical focal length \(F\) to simplify the analysis of the reference echo.

We employ a time coordinate system in which the center of the front-surface (FS) echo appears at \(t = 0\) when the waterpath is \(z_{0FS}\). In our case, we assume that the backscattered noise arises solely from single scattering of the incident beam by the individual metal grains. Then, our algorithm for calculating a “simulated” time domain noise signal contains the following steps: (1) specify the particulars of the pulse/echo inspection to be simulated, including information about both the measurement system and the material, (2) determine a time interval within which the noise calculation is to be valid, and an associated spatial region in the solid where all contributing grain will reside, (3) using random number generators, pick points in the spatial region to serve as grain centers, (4) assign a size to each grain, based on the proximity of its nearest neighbor and the conservation of volume, (5) using random number generators, orient the principal crystallographic axes of each grain, (6) using the ultrasonic measurement model of Thompson and Gray,\(^18\) calculate the (discrete) spectral amplitudes of the backscattered signal from each grain, (7) add up the contributions from all grains to determine the spectral amplitudes of the total noise signal, and (8) perform an inverse Fourier transform to obtain the time-domain total noise signal. The result of this process is a simulated total noise signal for “one ensemble” of grains (equivalent to one transducer position in a scanning experiment). The calculational algorithm is repeated many times to gather a sufficient number of independent total noise signals for statistical analysis.

The inputs for a Monte Carlo noise calculation consist of the usual geometric and material parameters, together with additional quantities to describe the microstructure. In the first group are the transducer focal length and radius, the waterpaths for reference and noise signal acquisition, the reference signal itself, and the density, sound speed, and attenuation of water and the metal. In the second group are the number of grains per unit volume \((n)\), the single crystal elastic constants in a principal axis coordinate system \((C_{ij})\), the material density, and distribution functions which describe the likelihood that a given grain has a particular size, shape, and orientation relative to the laboratory \((x_1,y_1,z_1)\) coordinate system. For the calculations described in this paper we explicitly consider only equiaxed, randomly oriented collections of grains, treated by making each grain spherical and by making each orientation of principal axes equally likely.

Since the noise calculation must be completed in a reasonable period of time and since computer memory limitations may apply, it is generally neither possible nor efficient to consider all grains in a physical specimen. Thus various strategies must be adopted to limit the number of grains which must be considered in a given ensemble. Our strategy has two parts. First we limit the time interval within which the calculation will be valid to a particular “time window of interest” (TWOI). This effectively imposes a restriction on the depths \((z_1)\) of the contributing grains. We then impose a restriction on the lateral coordinates \((x_1,y_1)\) by confining the grains to the region where the incident ultra-
sonic field is appreciable. The resulting volume in the metal into which the centers of model grains are placed is termed the ‘spatial region of interest’ (SROI). The relationship between the TWOI and the SROI is illustrated in Fig. 1. By definition, all grains whose centers lie in the SROI are capable of producing a backscattered echo which: (1) is appreciable in amplitude and (2) is totally or partially enclosed by the TWOI. Conversely, no grains outside of the SROI are likely to produce appreciable echoes in the TWOI.

If the grains are very small and the metal is only weakly attenuative, then the duration of a single-grain echo is approximately that of the front surface (FS) reference signal. For larger grains, the time delay between the front and back grain-boundary echoes may be appreciable and should be taken into account. In the latter case the minimum and maximum depths of the SROI and the starting and ending times of the TWOI are approximately related by

\[
t_{\text{min}} \sim \frac{2z_{1,\text{min}}}{v_1} + \frac{\Delta t_{\text{ref}}}{2} + \frac{d}{v_1},
\]

\[
t_{\text{max}} \sim \frac{2z_{1,\text{max}}}{v_1} - \frac{\Delta t_{\text{ref}}}{2} - \frac{d}{v_1},
\]

where \(\Delta t_{\text{ref}}\) is the duration of the reference signal, \(d\) is the average grain diameter, and \(v_1\) is the speed of sound in the metal. For some ensembles, grains of larger than average size will be located on the beam axis with the centers just inside the SROI, and these can further reduce the TWOI, if the incident field is strong at their location. Thus, in practice it is safer to replace \(d\) by 1.5\(d\) or 2\(d\) in Eqs. (1). Note that multiple reverberations within a grain have been neglected.

After tentatively choosing the depths \(z_{1,\text{min}}\) and \(z_{1,\text{max}}\), we limit the lateral extent of the SROI. This is done by considering the incident radiation pattern in the metal at each of several frequencies which span the range where the spectral components of the reference signal are appreciable. As a measure of the strength of the incident sonic field, we use the diffraction focussing factor \(C\) of Ref. 18 which is proportional to the ultrasonic displacement or velocity. Note that the magnitude of an echo from a small scatterer is proportional to \(|C|^2\) at the location of the scatterer. At each frequency we locate the peak value of the diffraction/focusing factor of the incident field \(|C|\) on the depth range of the SROI \((z_{1,\text{min}} \leq z \leq z_{1,\text{max}})\). Since a Gaussian beam model\(^{19}\) is used for all field calculations, this peak will always occur on the beam axis. We then determine the lateral boundaries of the spatial region within which \(|C| \leq c|C_{\text{max}}|\), where the cutoff factor \(c\) is typically chosen to be 0.01 or smaller. This can be done analytically because of the simplicity of the Gaussian beam expression for \(|C|\). The union of the volumes determined in this manner for the different frequencies is taken to be the SROI. The boundary of the SROI is generally determined by the radiation pattern at the lower frequencies. For a planar or spherically focused circular transducers at normal incidence, the SROI always has rotational symmetry about the beam axis. For a focused transducer, the SROI boundary often has a nozzle-like shape as shown in Fig. 2(a). In practice, we usually limit the number of grains occupying the SROI to 200 000 or fewer. For a given density of grains and transducer beam, this imposes a limitation on the depth of the SROI, and hence on the duration of the TWOI.

Once the boundary of the SROI has been determined, grain centers must be randomly placed within it. Such centers are chosen one at a time until the number within the SROI equals \(n\) times \(V_{\text{SROI}}\), where \(n\) is the input grain density and \(V_{\text{SROI}}\) is the volume of the SROI. Most computer systems have built in software for choosing a sequence of random real numbers which are uniformly distributed on \([0,1]\) and we make use of such software when assigning grain centers. For the case in which the grains are equiaxial and hence represented by sphere in our model, the following procedure is used to choose center points for one ensemble of grains: (1) The SROI is ‘enlarged’ by a small amount (> twice the mean grain diameter) in each direction. This is done for later convenience in determining nearest neighbors. (2) The enlarged SROI is covered by nonoverlapping cubes of identical size as shown in Fig. 2(b). (3) Grain centers are chosen one at a time by randomly choosing a cube; and randomly choosing a point in the cube. (4) If the point chosen in the last step lies within the enlarged SROI, its coordinates are stored in computer memory. Otherwise, the point is discarded. (5) The assignment of grain centers continues until there are \(nV_{\text{SROI}}\) centers located within the original (non-\(n\) enlarged) SROI. The number of centers within the enlarged

![FIG. 2. (a) Assignment of grain centers for one low-density simulation of a focused probe inspection. Here 900 grain centers have been determined and their projections onto the \(x_1z_1\) plane are shown. (b) When generating centers, the SROI is enlarged slightly and subdivided into cubes.](image-url)
SROI (which are stored in memory) will, of course, be somewhat higher. A similar procedure can be used to generate centers for the case in which the grains are nonspherical and have their shapes preferentially aligned with the $x_1$, $y_1$, and $z_1$ axes. In that case the enlarged SROI is divided into identical rectangular parallelepipeds with sides chosen proportional to the average projected grain diameter on the parallelepiped axes. The selection of grain center coordinates within a given parallelepiped is analogous to the equiaxed case: in each dimension the random numbers on [0,1] are linearly mapped onto the full length of the corresponding parallelepiped side. The effect is equivalent to randomly choosing a set of points within a cube and then deforming the cube into a parallelepiped: the average separation vector between nearest neighbors has different projections on the $x_1$, $y_1$, and $z_1$ axes.

Having determined the centers and enumerated them using an integral index $i$, other attributes such as size, shape, and orientation must be assigned to the grains. Depending upon the microstructure under consideration, these attributes could be assigned in an independent fashion using random number generators to select values that are distributed in a specified manner. For the spherical grain case considered in the present paper, we have chosen to determine grain sizes from nearest neighbor distances, rather than assigning them randomly. Very unphysical situations can occur if the sizes are randomly assigned: e.g., a large grain may completely enclose one or more of its smaller neighbors, or several small neighboring grains may occupy only a tiny fraction of the available local volume. Such gross improprieties are avoided by relating grain sizes to nearest-neighbor distances. In particular, for each grain $i$ in the (nrlarged) SROI, we locate the center-to-center distance to its nearest neighbor ($\tilde{r}_i$). The radius ($r_i$) of grain $i$ is then determined from: $r_i = b \tilde{r}_i$ where the constant of the proportionality (b) is fixed by the condition that the sum of the grain volumes be equal to the volume of the SROI. When locating the nearest neighbor of a given grain, all center points in the enlarged SROI are considered. The use of the expanded SROI allows a proper estimation of nearest-neighbor distances for grains that are located within but near the boundary of the original SROI. Because a hundred thousand or more grains are involved (and hence 10 billion or more possible pairs of grains) it is important to streamline the determination of nearest-neighbor distances. We begin by ordering the stored coordinates of the grain centers in all cubes according to their depth ($z_1$ coordinate) values. For each of several ranges of $z_1$, the coordinates are further ordered first by $x_1$ and then by $y_1$. Our search algorithm then makes use of this ordered storage format to rapidly determine the nearest neighbor of each grain. The approach here is similar to subdividing the enlarged SROI into many small cubes. To locate the nearest neighbor of a given grain center, only centers having similar $z_1$ coordinates and residing in the same or abutting cubes are examined. After the nearest-neighbor distances and grain radii are determined and stored, the grain centers located outside of the original SROI are discarded.

Our method of assigning sizes leads to a particular distribution of grain radii. The grain size distribution function $p(r,n)$ is defined by the condition that $p(r,n) dr$ equals the probability that the radius of an arbitrarily selected grain is between $r$ and $r+dr$ when there are $n$ grains per unit volume. For our grain-generation algorithm in the large-volume limit, one can show that the proportionality constant $b$ has the value unity, and that

$$p(r,n) = 4 \pi n r^2 \exp(-4 \pi n r^3/3) \quad (2)$$

in this limit. The mean grain diameter which appears in Eq. (1) is consequently

$$\bar{d} = \int_0^\infty 2 r p(r,n) dr = \frac{2 \Gamma(\frac{1}{3})}{(36 \pi n)^{1/3}} = 1.108 n^{-1/3} \quad (3)$$

and the most probable diameter, obtained from $dp(r,n)/dr = 0$, is

$$d_{\text{prob}} = \frac{2}{(2 \pi n)^{1/3}} = 1.084 n^{-1/3}. \quad (4)$$

Equations (2)–(4) are not required for MCM calculations. However, they are included since they define the particular distribution of grain sizes implied by our strategy, and their knowledge is often useful for testing purposes. Note that $b=1$ implies that each grain’s radius is equal to the center-to-center distance to its nearest neighbor, leading to substantial volume overlap between neighboring grains. Such volume overlaps balance the volume of the regions which are not enclosed by any grains.

For single-phase, spherical grains of a given material, the microstructural attributes which determine the backscattered signals are the locations and sizes of the grains, and the orientations of their principal symmetry axes. In our calculations the orientation of each grain is determined independently of the others by applying Euler rotations through randomly chosen angles. We begin with the principal axes of a given grain aligned with the $(x_1,y_1,z_1)$ “lab” axes, and we apply three successive active rotations to the grain: (i) a rotation through angle $\phi$ about the lab $z_1$ axis; (ii) a rotation through angle $\theta$ about the lab $y_1$ axis; and (iii) a rotation through angle $\psi$ about the lab $z_1$ axis. We desire that all final orientations of the principal axes be equally likely and this requires that three Euler angles be chosen such that $\phi$ is uniformly distributed on $[0,2\pi]$, $\cos \theta$ is uniformly distributed on $[-1,1]$, and $\psi$ is uniformly distributed on $[0,2\pi]$.

Once the necessary grain attributes have been assigned, the spectral components of the echo from each grain must be calculated. This is done using the ultrasonic measurement model of Thompson and Gray, which relates the measured echo to the farfield scattering amplitude of the grain. The measurement model calculation of the echo from one grain requires knowledge of the scattering amplitude for longitudinal-wave backscatter. As we shall see shortly, this scattering amplitude depends upon the $33$ (or $zz$) component of the grain’s elastic stiffness matrix in the lab coordinate system. This component, denoted here by $C''_{33}$ can be expressed in terms of the single-crystal elastic constants in a principal axis system ($C''_{jk}$) and the three Euler angles $(\phi,\theta,\psi)$ used to orient the grain. Using the transformation formulas for coordinate system rotations, we find that
by the size and shape of the scatterer. Here, all grains are taken to be that of any single grain, so

\[ k = \text{frequency} \]

where constants of the host medium are taken to be the Voigt averages of individual crystallites (mean stiffnesses under ‘‘constancy of strain’’), following the demonstration of Rose that this is the appropriate choice. Voigt-averaged elastic properties for equiaxial distributions of randomly oriented crystallites are available in the literature for our two cases of interest:

\[ (C_{33})_{\text{Voigt}} = (3C_{11} + 4C_{12} + 4C_{44})/5 \]

(cubic symmetry),

\[ (C_{33})_{\text{Voigt}} = (8C_{11} + 3C_{33} + 4C_{13} + 8C_{44})/15 \]

(hexagonal symmetry),

\[ v_{\text{host}} = \sqrt{(C_{33})_{\text{host}}/\rho_{\text{host}}} \]

As in Eqs. (5)–(6), the quantities on the right-hand sides of Eqs. (9)–(10) are single crystals elastic constants in a principal axis coordinate system. The quantity on the left-hand side of either equation is the Voigt-averaged isotropic stiffness whose value is to be substituted for \( C_{33} \) in \( \delta C_{33}/C_{\text{host}} \). In addition, the density of the averaged medium is naturally taken to be that of any single grain, so \( \delta \rho = 0 \) is used in Eq. (7).

Having described the assignment of grain locations, sizes, orientations, and scattering amplitudes, it is now a straightforward exercise to calculate the backscattered echoes from each grain using the measurement model. The Fourier transform of the reference signal at angular frequency \( \omega \) is written as

\[ R(\omega) = \beta(\omega)R_{00}D(\omega)\exp\left(-2i(k_0z_{0R} - 2\alpha_0z_{0R})\right) \]

and the Fourier transform of the voltage signal observed in the noise measurement geometry due to direct scattering by a single anisotropic grain located at position \((x_1, y_1, z_1)\) in the solid is written

\[ \delta S(\omega, x, y, z) = \left[2\beta(\omega)A(\omega)\rho_1v_1\right]/(i(k_1^2a_1^2 \rho_0v_0)] \times T_{01}C^2(\omega, x_1, y_1, z_1)\exp[-2i(k_0z_{0S} + k_1z_{1S}) - 2(\alpha_0z_{0S} + \alpha_1z_{1S})]. \]

In Eqs. (12)–(13), the host polycrystal is treated as an attenuative isotropic medium. The symbols \( \nu, k, \rho, \alpha, \) and \( a \) denote longitudinal wave velocity, wave number \((k = \omega/v)\), density, attenuation constant, and transducer radius, respectively. Subscripts 0 and 1 refer to water and solid, respectively, and subscripts \( R \) and \( S \) refer to the reference and noise geometries which may have different waterpaths. \( \beta \) is the transducer efficiency, which can be expressed in terms of the reference signal amplitude \( R(\omega) \) using Eq. (12). \( R_{00} \) and \( T_{01} \) are plane-wave reflection and transmission coefficients. \( C(\omega, x_1, y_1, z_1) \) is a measure of the incident ultrasonic field strength in the metal after adjusting for interface transmission and attenuation. \( D(\omega) \) accounts for the effects of diffraction losses in the reference signal. The waterpath \((z_{0R} \text{ or } z_{0S}) \) is measured outward from the transducer face along the central ray direction. Finally, \( A(\omega) \) is the scattering amplitude for backscattered sound from the grain in question as given in Eqs. (7)–(8). The Lommel diffraction correction \( D \) is calculated using the analytic expression of Rogers and Van Buren which was derived for planar transducers. The negative of the complex conjugate of their expression also gives the diffraction correction for a focused transducer when the reflecting plane is located at geometric focus. The incident displacement field in the metal, \( C \), is calculated using the Gaussian beam model of Thompson and Lopes. Explicit expressions for all quantities appearing in Eqs. (12)–(13) can be found in Ref. 20.

Note that we could simply use Eqs. (12)–(13) to directly calculate the time-domain echo from each grain, and then sum these to obtain the total noise signal for the ensemble of grains. Rather than doing this, we adopt a distinct but equivalent approach which makes more efficient use of the measurement model formulas: we perform the sum over grains in the frequency domain rather than in the time domain. At each (discrete) frequency in the bandwidth of the input (discrete) reference signal, we calculate the spectral amplitude of the echo from each grain, and then sum these to obtain the amplitude of the total noise signal. After all spectral amplitudes of the total noise signal have been computed, we perform an inverse Fourier transform to obtain the time-domain representation of the signal. This approach avoids needless multiple inverse Fourier transform operations.
The total noise echo from all 502 grains in the ensemble is and distinct echoes from its front and back walls can be seen. The attenuation at each frequency was assumed to be zero. In panel (c) we display the backscattered echo from a single, hexagonal crystal structure of diameter 0.8 cm and extends 0.4 cm in the focal zone of the transducer. Calculated backscattered echoes from (c) one grain, and (d) one ensemble of grains are shown.

C. Outputs of the model

Selected results from one Monte Carlo calculation are shown in Fig. 3. There we have assumed a specimen of alpha-phase titanium (hexagonal crystal structure: \( v_f = 0.601 \text{ cm/\mu s} \), \( \rho_f = 4.54 \text{ g/cm}^3 \)) containing \( n = 1000 \) grains per cubic centimeter. The single crystal elastic constants were taken from Ref. 24, namely \( C_{11} = 160 \), \( C_{12} = 90 \), \( C_{13} = 66 \), \( C_{33} = 181 \), \( C_{44} = 46.5 \), and \( C_{66} = 35 \) in GPa units. We assumed that the specimen was insonified using a 15-MHz toneburst pulse emitted from a focused transducer having a radius of 0.64 cm and a geometric focal length of 9.49 cm. The assumed waterpaths are 9.65 and 6.0 cm for reference signal acquisition, respectively. The SROI is a disk-shaped region of diameter 0.8 cm and extends 0.4 cm centered in the focal zone of the transducer, its volume is 0.502 cm³. The corresponding SROI is shown in Fig. 3. The discretized reference signal [Fig. 3(a)] was a measured front-surface echo containing 1024 points at a sampling rate of 100 MHz, leading to a discrete Fourier spectrum with a stepsize of \( \Delta f = 1/(1024 \Delta t) = 0.098 \text{ MHz} \) [Fig. 3(b)]. To limit computation times, explicit calculations were performed only at each of the 42 discrete frequencies in the range 13 MHz \( \leq f \leq 17 \text{ MHz} \), and the effective metal attenuation at each frequency was assumed to be zero. In panel (c) of Fig. 3 we display the backscattered echo from a single, larger-than-average grain located in the portion of the SROI nearest the transducer. This grain has a diameter of 0.14 cm and distinct echoes from its front and back walls can be seen. The total noise echo from all 502 grains in the ensemble is shown in panel (d). Notice in both panels that the calculated signal is very small at early and late times, indicating that errors arising from spectrum truncation are minimal.20

D. Test of the model

It is illuminating to compare the predictions of the Monte Carlo noise model with experiment. Such a comparison is practical if the number of grains in an ensemble is not so high as to tax the capabilities of the computing system. Of the specimens having single-phase, equiaxed, randomly oriented microstructures at our disposal, a copper specimen had the largest mean grain size, and hence was the best candidate for study. An experiment was performed to measure average and peak noise levels for this specimen using broadband incident sound pulses having a center frequency near 5 MHz. A focused transducer having a measured radius of 0.64 cm and a measured geometric focal length of 9.49 cm was used, and backscattered noise echoes were recorded at 100 transducer positions. Based on an analysis of the depth dependence of backscattered noise,20 we suspected that multiple scattering effects may be significant in this specimen, particularly above 5 MHz. Thus we used the lowest-frequency transducer available that had acceptable focusing properties. (Focusing was desirable to limit the size of the SROI, and hence to limit the number of grains in a model ensemble.) In addition, we chose the waterpath relatively long so that the focal region under study was near the metal surface and produced noise echoes at early times where multiple scattering effects are expected to be smaller.10 In particular, with a specimen velocity of \( v_f = 0.472 \text{ cm/\mu s} \) and a waterpath of \( z_{0.5} = 7.2 \text{ cm} \), the geometric focus was located 0.72 cm beneath the water/metal interface, and the round-trip travel time from the interface to the focus was 3.0 \( \mu \text{s} \). Our intention was to compare measured noise attributes on the interval 1.5 \( \mu \text{s} \leq t \leq 4.5 \mu \text{s} \) with the predictions of the MCM, and time-domain noise echoes were measured at 100 transducer positions. In addition to the noise signals, the standard FS echo was recorded at a waterpath of \( z_{0.8} = \text{focal length} = 9.49 \text{ cm} \). The measured broadband reference signal and the spectrum are shown in Fig. 4.

Noise signal prediction using the Monte Carlo model requires an appropriate input value for the grain density \( n \). To estimate \( n \), we analyzed a micrograph showing the grain structure of the test specimen, and we determined \( P(L) \) the probability that a line segment of length \( L \) placed arbitrarily on the photo has both ends inside of one grain. Our procedure for measuring \( P(L) \) is described in detail in Ref. 20. The measured \( P(L) \) function was then compared to the corresponding functions for model ensembles of spherical grains with different densities. Using the size distribution function for the spherical grains as given in Eq. (2), the probability that a line segment of length \( L \) has both ends inside of one grain may be calculated20

\[
P(L,n) = \exp(-\pi n L^2/6) - (\pi n L^3/6)^3 \Gamma(2/3,2\pi n L^3/3)
\]

(14)

for a large MCM model ensemble of spherical grains with number density \( n \). Here \( \Gamma(a,x) \) denotes the incomplete Gamma function. Figure 5 compares the \( P(L) \) function de-
duced from the photographic analysis of our copper specimen with the model $P(L,n)$ for three choices of $n$. Model and experiment are seen to be in reasonable agreement when $n = 100,000$ grains per cubic cm is assumed in the MCM. The level of agreement is far from ideal, however, indicating that the distributions of grain sizes are somewhat different in the specimen and the model ensemble. Nonetheless, $n = 100,000$ appears to be reasonable choice when applying the MCM to the copper specimen.

The MCM calculation of synthetic noise echoes requires as an input the longitudinal ultrasonic attenuation coefficient $\alpha_1$ of the test specimen. Two separate experimental methods were used to measure this attenuation, with differing results. $\alpha_1 = 0.05 f^{1.2}$ nepers/cm for $2 \, \text{MHz} \leq f \leq 5 \, \text{MHz}$ resulted from an analysis of the depth dependence of backscattered noise in a series of measurements with different water-paths and hence different metal depths to the focal zone, and $\alpha_1 = 0.01 f^{2.5}$ nepers/cm for $1 \, \text{MHz} \leq f \leq 7 \, \text{MHz}$ was determined by deconvolving front and back surface echoes in immersion inspections using planar transducers (both measurement methods are described in Ref. 9 and results for each method are described in Ref. 20). We decided to perform MCM calculations for both choices of the attenuation function.

For the MCM predictions of synthetic noise echoes for copper, the model SROI was a disk of diameter 1.8 cm centered near the geometric focus in the experiment and extending over $0.3 \, \text{cm} \leq z_1 \leq 1.1 \, \text{cm}$. It contained 204,000 model grains per ensemble at the assumed density $n = 100,000$ grains/cm$^3$. The associated TWOI in which the noise calculations were valid was $1.7 \, \mu s \leq t \leq 4.2 \, \mu s$. The input reference signal contained 512 time points at a 100-MHz sampling rate, and calculations were performed for each of the 57 discrete frequencies on $0.98 \, \text{MHz} \leq f \leq 11.91 \, \text{MHz}$. The single-crystal elastic constants for copper were taken from Ref. 26, namely $C_{11} = 169$ GPa, $C_{12} = 122$ GPa, and $C_{44} = 75.3$ GPa. For each choice of $\alpha_1$, approximately 7 h of computation time on a DECStation-5000 machine was required for generation of simulated noise signals for 100 grain ensembles. The simulated and measured noise signals were then analyzed to determine the (absolute) rms noise level and the absolute peak (positive) noise voltage observed at each time instant in the TWOI, i.e., at a given time instant (say $t = 3 \, \mu s$) each of the 100 measured or simulated waveforms was evaluated to determine a set of 100 voltage values. The rms value of these 100 voltages and the peak positive voltage in the set were then recorded. These quantities are compared in Fig. 6. The measured rms noise level is seen to be in good agreement with theory, and indeed is bracketed by the predictions for the two choices of attenuation. The MCM also does a good job of predicting the dimensionless ratio of peak noise to rms noise. The predicted ratio is approximately independent of the choice of attenuation function, is relatively
constant in time, and its average value within the TWOI is very close to that seen in experiment. The measured ratio appears to fluctuate with a longer period than theory predicts, indicating that peak noise values at neighboring time points are more correlated with each other than is predicted. This discrepancy may be associated with the small physical size of the specimen. In order to obtain 100 measured noise signals it was necessary to scan the transducer in a rectangular pattern using an average stepsize of 0.2 cm which is considerably less than the mean diameter of the beam in the SROI (~0.8 cm). This circumstance may be responsible for the greater time coherence seen in the experimental peak noise data. Overall, the MCM does an excellent job of predicting the rms and peak noise levels seen in the copper specimen. This is particularly impressive because the predicted absolute noise signals are ~70 dB below the input front-surface reference signal, and no adjustable parameters are involved in the calculation.

II. MODEL APPLICATIONS
A. Comparison to other models explicitly based on microstructure

One possible use of the Monte Carlo model is to test other single-scattering models and techniques for noise signal analysis. The independent scatterer model (ISM), for example, predicts the rms average noise level from the measurement system parameters and the microstructural quantity $n^{1/2}/A_{\text{rms}}$, which is known as the ‘figure-of-merit’ (FOM). In the following example, we have used the MCM to predict backscattered noise echoes from an α-phase titanium specimen insonified with a 15-MHz toneburst from a focused transducer ($a=0.607$ cm and $F=9.65$ cm). The assumed reference signal, SROI and TWOI are the same as those described earlier in Sec. I.C. For each of seven choices of the grain density, 500 synthetic noise waveforms were calculated using the MCM, and from these the rms noise level was determined as a function of time. The predictions of the Monte Carlo and independent scatterer models are compared in Fig. 7. In each case the rms noise voltages have been normalized by dividing by one half of the peak-to-peak voltage of the reference signal. Good agreement is seen between the two models. Although, the average noise levels are seen in Fig. 7 to increase with increasing grain density, the rms noise level is expected to drop with further increase in grain density at some point. It should be recognized that this trend will not continue for arbitrarily large densities, since in that limit, the material is a continuum. Instead a plot of noise versus grain density will show a maximum, followed by a decrease at large values of the density. Analogous behavior has been shown for the scattering component of attenuation.

B. Distribution of noise voltages

If we confine attention to a single time instant after the front-surface echo (or a time window of short duration), and record the noise voltage for many ensembles, the resulting distribution of voltages is expected to have a mean value of zero in the absence of any instrumentation background. The precise manner in which the voltages are distributed about this mean is found to depend upon the density of grains. Generally speaking, only a small percentage of the insonified grains have the proper combination of location, size, and orientation to produce a large backscattered signal. When the density of grains is large, however, there will be many contributing, independent, appreciable echoes. In such a case, the central limit theorem applies, and one expects the total noise voltages to be distributed in a Gaussian manner about their mean. This behavior is seen at large $n$ for the simulated total noise voltages calculated in our MCM treatment of alpha-titanium. For example, as shown in Fig. 8(b), the voltage distribution is essentially Gaussian when $n=100,000$ grains/cm$^3$. However, the distribution can be markedly non-Gaussian for large-grained specimens as shown in Fig. 8(a). When the beam is focused and the grain density is small (i.e., <10,000 grains/cm$^3$ in this case) relatively few grains produce appreciable backscattered signals. One then finds more total noise voltages near zero than would be expected for a Gaussian distribution, and more voltages far removed from the mean (Fig. 9). Those noise voltages which are many standard deviations from the mean could easily be mistaken for defect signals if the flaw-detection threshold is based upon Gaussian analysis. The MCM results of Fig. 8 were obtained by binning the synthetic noise voltages observed for 500 ensembles; all voltages seen within a time interval of duration of 0.5 µs centered in the TWOI of Fig. 3 were binned.

The ratio of peak noise to rms noise, averaged over a time window to reduce point-to-point fluctuations, can be used to track the progression toward Gaussian behavior with increasing $n$. Figure 10 shows MCM determinations of this averaged ratio for seven choices of grain density in our focused-probe treatment of alpha-phase titanium. At each density the ratio has been calculated for each of five distinct collections of 100 ensembles. At a given time instant the expected ratio of peak noise to rms noise for 100 independent ensembles is 2.46 if the voltages are distributed in a Gaussian fashion. This value is shown by the solid line in Fig. 10. As the grain density increases, the averaged ratio calculated using the MCM is seen to approach the Gaussian result from above.
The relationship between the rms average noise and the peak noise seen during an inspection is a topic of ongoing study. Closely related is the question of how rapidly the noise waveform changes when the transducer is scanned. When two transducer positions are separated by a small distance, \( \Delta x \), the backscattered noise signals seen at the two positions may be correlated. Predictions of the degree of correlation can be made in a straightforward manner using the MCM. One enlarges the SROI in a lateral direction (e.g., along \( +x_i \)) so that the beam remains within the SROI while the transducer is scanned. The same ensemble of grains is used at each transducer position, however, the grain centers effectively shift with respect to the beam center as the transducer is scanned. For each ensemble, the total backscattered noise signal is calculated for a sequence of transducer positions, and the correlation coefficient for each pair of noise signals is found. This process is repeated for many ensembles to obtain stable average values. The results from one such series of MCM calculations is shown in Fig. 11 where we display the averaged correlation coefficient as a function of transducer separation for the same alpha-titanium inspection scenario considered earlier. In this case the envelope function (analytic signal of Ref. 32) of each rapidly oscillating noise waveform has been computed at each point in the TWOI and the vertical axis of the figure displays the averaged standard linear correlation coefficient for a pair of envelope functions. More specifically, if \( \{E_a(t_i); i=1,2,\ldots,m\} \)

FIG. 8. Grain noise voltage distributions resulting from MCM simulations of a focused-probe, toneburst inspection of alpha-titanium are shown for (a) \( n=100 \) grains/cm\(^2\), and (b) \( n=100,000 \) grains/cm\(^2\). Gaussian distributions having the same mean and standard deviation are also shown.

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FIG. 9. Positive tails of the voltage probability distributions shown in Fig. 8(a) for \( n=100 \) grains/cm\(^2\). A small but significant fraction of the measured voltages are further than 5 standard deviations from the mean.

FIG. 10. Ratio of peak noise to rms noise observed in MCM simulations of alpha-titanium inspections, for various choices of the grain density. For each group of 100 ensembles, the ratio has been calculated at each time instant and then averaged over an interval of duration 0.5 \( \mu s \) centered in the TWOI.

FIG. 11. Correlation between envelope functions of simulated noise waveforms at nearby transducer positions, for three choices of grain density in alpha-phase titanium.
denotes the discrete values of the noise voltage envelope function observed at transducer position \( a \), and \( \{ E_b(t) \} \) are the values nearby transducer position \( b \), then the quantity displayed on the vertical axis in Fig. 11 is

\[
\langle \text{Cor. Coef.} \rangle = \left( \frac{\sum_{i=1}^{m} (E_a(t_i) - \bar{E}_a)(E_b(t_i) - \bar{E}_b)}{\left( \sum_{i=1}^{m} (E_a(t_i) - \bar{E}_a)^2 \right)^{1/2} \left( \sum_{i=1}^{m} (E_b(t_i) - \bar{E}_b)^2 \right)^{1/2}} \right),
\]

where \( \bar{E}_a \) denotes the average of the \( E_a(t_i) \) within the TROI, and where \( \langle \cdot \rangle \) denotes the average over the 500 ensembles. One expects that the correlation-versus-transducer-shift function should depend upon the width of the beam in the SROI. Figure 11 indicates that it also depends upon the density of grains, suggesting that a measurement of the function could be used to ultrasonically estimate grain density in coarse-grained specimens. For the simulation shown here, the diameter of the incident beam near the focal zone is approximately 0.08 cm at -6 dB level, i.e., the amplitude of an echo from a point scatterer would be less than 6 dB below its peak (on-axis) value within this diameter.

C. Comparison of theories based on random walks and \( K \) distributions

The output of the Monte Carlo model has also been compared to predictions of a model based on the theory of random walks and the assumption that the distributions of backscattered echoes from individual grains follows a \( K \) distribution. The successful comparison, establishing an explicit link between the parameters of the microstructure and the \( K \) distribution, is discussed in a preliminary form in Ref. 33. References 34 and 35 describe a comparison of the latter theory to the various experimentally observed statistical characteristics of backscattered noise in titanium alloys, including non-Gaussian behavior of the unrectified signals. These preliminary accounts\(^{33-35}\) will be described in more detail in subsequent publications.

In addition, the MCM can be used to test simpler, approximate models, such as the ISM, which are more likely to be used in practical settings. The ISM essentially predicts the second moment of the distribution of noise voltages (the first moment being zero in the absence of instrumentation background). It would be of immense practical use to have similar, simple yet reasonably accurate, formulas which could be used to predict the full distribution of noise voltages or noise envelope values likely to be seen in a scanned inspection. MCM calculations can be used to guide the development of such formulas and to test their validity.

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