Mechanistic Understanding of Material Detachment During Micro-Scale Polishing

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Abstract
A combined experimental and modeling approach has been devised to understand the material removal mechanism during abrasion of ductile copper discs. First, single grit scratch intersection experiments are conducted at the micro-scale (with 1-30 mm depth of cut). This is followed by FEM analysis. Then a simple analytical model is developed, and the model prediction is verified against experimental observations and results from numerical simulations. A characteristic material detachment length is correlated between experimental observations and model predictions. The insights gained from this exercise may be used to develop a mechanistic model of material removal in chemical mechanical polishing (CMP) of ductile materials.

Disciplines
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A combined experimental and modeling approach has been devised to understand the material removal mechanism during abrasion of ductile copper discs. First, single grid scratch intersection experiments are conducted at the micro-scale (with 1-30 μm depth of cut). This is followed by FEM analysis. Then a simple analytical model is developed, and the model prediction is verified against experimental observations and results from numerical simulations. A characteristic material detachment length is correlated between experimental observations and model predictions. The insights gained from this exercise may be used to develop a mechanistic model of material removal in chemical mechanical polishing (CMP) of ductile materials. [DOI: 10.1115/1.1619964]

1 Introduction

Precision finishing is becoming an integral processing step in multilevel metallization designs for integrated circuit (IC) manufacturing. This is needed to ensure local and global surface planarization before the next layer is deposited. The surface finishing process (industrially known as Chemical-Mechanical Polishing, CMP), employ micro and nano particle abrasives in chemically active slurry with a soft polishing pad to remove material from the surface. The chemical aspect of the process is thought to be softening or dissolving the top layer of the surface while mechanically removing it. This work focuses on understanding the mechanical aspect of the surface material detachment mechanisms during the CMP process. The experimentally observed deformation patterns and force profiles from the micro-scale scratch experiments are used to provide a plausible mechanism for material detachment through a combination of surface plowing and shearing under the abrasive particles. The gained insights can be integrated into mechanism-based models for the material removal rate (MRR).

The process of mechanical surface polishing is usually envisioned through the phenomenological Preston formula [1]; wherein

\[
\frac{dH}{dt} = C^*P^*U, \tag{1a}
\]

where \(P\) is the applied down pressure, \(U\) is the relative sliding velocity and \(C\) is a proportionality constant. The volumetric material removal rate is given by

\[
MRR = A^*\frac{dH}{dt}, \tag{1b}
\]

where \(H\) is the height removed and \(A\) is the wafer area. All the unforeseen process parameters are lumped into the proportionality constant. Detailed analysis [2–4] have shown that the pressure dependence is nonlinear with exponent that ranges from 0.33 to 1.2 based on the details embraced by the model. These models also overestimate the MRR by several orders of magnitude. Such discrepancy is normally compensated by adjusting the proportionality constant (called Preston constant) in the equation.

All of the existing polishing models assume that each particle under the applied load generates a continuous trench, and the material removed is equated to the volume of this trench. Such a model is applicable at the macro-scale and is in agreement with the conventional card model [5] used in metal cutting.

It is hypothesized in this paper, that the material removal mechanism at the micro- and nano-scale is different. At these very small depths of cut, the abrasive particle forms a continuous trench, but the material is not detached from its parent surface. It merely flows from the bottom of the trench to the side via stable plastic deformation. Such deformation pattern has been observed in nano-scale AFM indentation and scratch tests [6,7], and is akin to profile rolling of gears [8,9]. It is further hypothesized that detachment occurs later as a result of plastic instability due to interaction of scratches. This interaction may be in the form of intersection of two scratches may be due to the vicinity of two parallel scratch-tracks [7]. It can also result from metal fatigue due to repeated plastic deformation in the pile-up region beside the trenches produced by the abrasive particles.

Here, only a particular form of this interaction—that due to normal intersection of scratches is considered. The experimental observations are presented next. This is followed by FEM analysis. Then a simple analytical model is constructed to capture the salient features of this phenomenon.

2 Experiment

A micro-scratch experimental setup (Fig. 1) is devised around a high precision rotational spindle to provide controlled scratch. The setup has two piezoelectric load cells (PCB-model 208C01, 101b capacity) for measuring the applied normal and tangential forces. The specimen post has rotational degrees of freedom about z-axis to provide control of the intersecting scratches. A conical diamond indenter with included angle of 90° and a tip radius of approximately 5 μm is utilized. The surface scratch is generated by rotating the spindle with the indenter around an axis parallel to the surface. The scratch depth is controlled by moving the specimen holder relative to the indenter tip. The force profiles are recorded with a dynamic DAQ system (ACE model DP104 FFT Analyzer, 20 kHz bandwidth). The whole test lasts approximately 40 ms to generate a 2 mm scratch length. The selected test parameters provide approximately a data point for every 2 μm of the scratch length.

Oxygen free, 99.99% high purity copper (101-alloy series) discs are utilized. The discs are ground and polished with 3, 1 and 0.05 μm alumina particles, respectively. A primary scratch is applied to the surface first. Then, the specimen is polished again to remove the pile up around the formed scratches. In several cases, this step resulted in a recess around the scratch sides, as will be seen in the force profile. The specimen is mounted back to the
testing setup, while repositioning the primary scratch at a 90° angle relative to the incoming one. A secondary scratch is then applied to intersect with the primary one. The testing procedure is repeated for a scratch depth in the range of 1–30 µm. Since the scratch track follows a circular arc, the exact depths of both scratches are measured by a surface profilometer at their point of intersection. Figures 2(a) and (b) show the SEM images of the intersecting scratches. Within the shearing zone, dimpling is visible as an indication of plastic tearing near the intersection zone.

2.1 Experimental Results. A typical force-time diagram for the secondary scratch is shown in Fig. 3(a) for three intersections. On this plot “positive” represents the normal indenter force, \( F_n \) and “negative” represents the tangential force, \( F_t \). The multiple ripples on the force curve are due to the dynamic response of the specimen fixture after indenter tip unloading/reloading at the intersection. However, these frequencies have distinctively different characteristic wavelength relative to those of the intersecting scratches. The ratio of \( F_t/F_n \) is approximately 0.3–0.4. The details of the tangential forces of scratch No. 2 is shown in Fig. 3(b). Several rates of the tangential force decays can be observed. Starting form the steady state ploughing process and approaching the primary scratch, \( F_t \) starts to drop slowly, following the recess near the primary scratch, which was induced by previous polishing. Up to this point, the material is ploughed. Then, \( F_t \) decays at a faster rate, which we termed “a transition to shearing action.” As the sheared segment collapses into the primary scratch, the decay rates drop until the sheared (or extruded) segment makes full contact with the other side of the primary scratch and subsequently \( F_t \) starts to rise again. The length of the sheared segment \( \ell \) is consistently measured for all tested cases and is plotted against the scratch depth of the secondary scratch at the point of intersection, \( h \), in Fig. 4. It is found that \( \ell \) is approximately 3.7 times \( h \).

In a realistic polishing process, pile-ups along the primary scratch will be present. In our experiments, we detected the onset of detachment due to secondary scratching by monitoring the drop in \( F_t \). Since, pile-ups from primary scratches would modify \( F_t \) according to the shape of the pile-up, it would introduce another variable influencing \( F_t \). Hence, presence of pile-ups would have made it more difficult to draw meaningful inferences from our measurements. We avoided this complication by eliminating pile-ups from primary scratches prior to secondary scratching.

3 Finite Element Simulation

The intersecting scratch concept for the material detachment mechanism is examined by FEM simulation using ABAQUS/Explicit [10]. The implemented 2-D plane strain model is shown in Fig. 5(a), where a recess in the surface is made ahead of the abrasive particle and equal to the initial depth of cut to simulate the interaction with the primary scratch. The abrasive particle is assumed rigid while the ploughed surface has material parameters consistent to those of copper (\( E = 109.2 \) GPa, \( \sigma_u \approx 69 \) MPa, \( \sigma_{ul} \approx 258.2 \) MPa). An isotropic elastoplastic strain hardening material model is used with hardening exponent \( n = 0.2 \). No friction is considered between the particle and the substrate. The simulation proceeded by translating the particle horizontally at a constant speed of 0.1 m/s, while preventing the vertical and rotational movements. Typical reaction forces on the abrasive particles are shown on Fig. 5(b) against the sliding distance for a depth of cut of 10 nm. Away from the surface recess, the ratio of \( F_t/F_n \) is approximately 0.37. The normal reaction \( F_n \) starts to drop at a distance of approximately three times the depth of the indentation, however, the decay of \( F_t \) was not observed. This may be due to the fact that shear localization takes place in the experiment along the inclined walls of the channel intended to be created by the abrasive particle, but that phenomenon was not captured by the FEM model. Utilization of cohesive elements with traction-separation law is expected to provide such capability of depicting the decay in the tangential force. Estimating the length of the “ejected piece” from the plot of the normal force \( F_n \), we arrive at: \( \ell \approx 3–4h \).

The FEM calculations use a cylindrical indenter in plane strain
radius 50 nm) with a depth of cut of 10 nm, while the experiments have used a conical indenter with nose radius of 5 μm, with a depth of cut range of 1–25 μm. Accordingly, differences between experiments and FEM predictions may be expected. It has been reported in literature [11], that depth of cut/nose radius essentially controls the relative magnitude of $F_t$ (normalized). Here, this ratio is 0.2 in FEM calculations, and vary from 0.2–5.0 for experiments. Accordingly, FEM results for 1 may be compared to only those experimental data where the depth of cut is around 1 μm.

4 Analytical Model Development

As observed from the scratch intersection experiments, both $F_t$ and $F_n$ starts to drop before the indenter creating the secondary scratch reaches the edge of the primary (pre-existing) scratch. The analytical model attempts to capture this phenomenon in a simple model.

It is envisioned that the deformation mode changes as the indenter approaches the edge of the primary scratch. When the indenter is far away from the edge, the material below the indenter is deformed, as in profile rolling, to form the pile up. It is assumed that this stable plastic deformation mode changes when the dis-

Fig. 3 (a) Normal and tangential forces for the secondary scratch. (b) Details of the tangential force close to the intersection zone, "2" showing different force decay rates.

Fig. 4 Characteristic length variation with the scratch depth

Fig. 5 (a) FEM abrasive particle-surface interaction model. (b) Normal and tangential reaction forces on the abrasive particle, showing the start of force decay at a characteristic distance from the primary scratch.
tance between the indenter and the edge drops below a critical threshold. At that instant, shear instability develops, and a piece of material is ejected from the scratch. The length of this piece is called the “characteristic length” of the material in our model development. The volume of this piece is the volume of material removed per intersection. The total MRR may then be estimated by estimating the number of such intersections per unit time.

4.1 Estimation of Tangential Force $F_t$ on the Indenter. The intent of this work is to eventually develop a model for MRR prediction in a nano-scale polishing or CMP process. In a typical polishing process, the down pressure is known. Utilizing the approach of [2–4], and determining the contact regime (no contact, partial contact or full contact between pad and wafer), the normal force $F_n$ per abrasive particle may be determined. In our current experimentation, the indenter represents a single abrasive particle, and the normal force $F_n$ on it will be known from process conditions. Knowing $F_n$, $F_t$ can be estimated using orthogonal metal cutting theory [5].

Referring to Fig. 6, we may write

$$F_t = F_n \cos \phi - F_n \sin \phi$$

When $F_t$ is the shear force on the shear plane and $\phi$ is the shear angle. Assuming a perfectly plastic material, we may estimate $F_t$ to be

$$F_t = \frac{\tau_{flow} \cdot A_s}{\sin \phi} \frac{wh}{\sin \phi}$$

When $\tau_{flow}$ is the shear flow strength of the material, $w$ is the width of cut and $h$ is the depth of cut, and $A_s$ is the area of the shear plane. Then $F_t$ may be expressed as

$$F_t = \frac{\tau_{flow} \cdot wh}{\sin \phi} + F_n \sin \phi$$

An iterative method may be used to determine the tangential force.

Iteration steps:

1. Use experimentally determined $F_n$. Alternatively, $F_n$ may also be estimated as normal force per particle from the prescribed down pressure in a polishing process.
2. Assume a shear angle value, (usually within $10^\circ$ to $25^\circ$).
3. Find $F_t$ value based on Eq. (4).
4. Find the $F_t/F_n$ ratio.

5. Find the friction angle on the chip-tool plane as,

$$\beta = \tan^{-1} \left( \frac{F_t}{F_n - \tan \alpha} \right),$$

where $\alpha$ is the rake angle.

6. Obtain shear angle $\phi$ based on the principle of minimum energy.

$$\phi = \left( \frac{\pi}{4} + \frac{\alpha}{2} \right) - \frac{\beta}{2}$$

and check for convergence of shear angle $\phi$.

Experimental values: $h = 12 \mu m$, $\alpha = 45^\circ$, $F_n = 2.5N$, $F_i = 1.22N$.

The $F_i$ value when convergence of $\phi$ is obtained is the desired estimate of the tangential force during the scratching process when the indenter of the tool is far away from the edge of the primary scratch. This $F_i$ value represents the maximum $F_i$ that can be supported by a perfectly plastic material before the material will fail at the shear plane.

As an intermediate check, we compared the experimental $F_i$ value to the estimate of $F_i$. Table 1 shows the comparison for different assumptions. $\tau_{flow}$ can be assumed to be either the initial shear yield strength or the shear ultimate strength of copper. To be consistent with plane strain assumption in orthogonal metal cutting theory, $w$ should be large compared to $h$. However, in the experiment, it is a conical indenter with an included angle of $90^\circ$. So $w$ may be estimated as $w = 2h \tan(\alpha)$ or $w = 2h$ for this indenter. However, adopting (3) and for $\tau_{flow} = \tau_{ult} = 220/\sqrt{3} MPa$, the estimated $F_i$ matches the experimentally evaluated one for approximately $w = 10h$ in the model. Such estimates are adopted for later calculation.

4.2 Material Detachment Model. Referring to Fig. 6, we propose a very simple shear failure mechanism, where shear failure occurs along a horizontal plane extending from the indenter to the edge of the primary scratch before shear localization can take place according to traditional metal cutting theory. Then

$$F_i = \frac{\tau_{flow} \cdot w \cdot \ell}{\cos \phi}$$

Assuming $\tau_{flow} = 220/\sqrt{3}$ and $w = 10h$ for $h = 12 \mu m$, we get $\ell = 7.6h$ for $F_i = 1.4N$. This higher value of $\ell$ may be due to the fact that only the bottom plane, and not the entire shearing area has been considered in the above simple analytical model.

5 Discussion

The scratch intersection experiment has provided a plausible mechanism of material removal during surface finishing process for ductile material under small depth of cut and light load. In
spite of the fact that the material is ploughed to the trench sides by the abrasive particles, however, a segment with a characteristic length, \( \ell \), is sheared off from the formed trench, whenever two trenches intersect each other at right angle. Such characteristic length is found to be approximately 3–4 times indentation depth, which is also justified by FEM analysis. However, several points should be noted:

1. Our results are valid for 99.99% annealed copper we tested. The characteristic detachment length could be different for other materials with different properties, particularly for those with different work hardening characteristics.

2. The orthogonal intersection of scratches is chosen to identify the material detachment phenomenon. The intersections at other angles need further investigation.

3. The model we propose here is a “particle scale” model, where we focus on the material detachment mechanism due to a single abrasive particle. The input parameters are normal and tangential forces on a single particle. The interface pressure in a CMP process may indeed vary, and become suction pressure at certain location. Accordingly, the normal and tangential forces on the abrasive particle will need to be adjusted.

The simple shear failure criterion used in the analytical model predicts \( \ell \) to be around \( 7.6h \) for the experimental conditions on copper, which is of the same order, but still significantly higher than the experimental value. There may be several reasons for this discrepancy:

1. Only the shear failure along the bottom plane is considered in the analytical model. For the conical indenter in the experiment, the surface of shear failure may be inclined and different.

2. The assumption \( w = 10h \) to represent plane strain is approximate.

3. The material may be strain hardening due to the deformation induced by the scratching process, while only a perfect plasticity assumption is used in the present analytical model.

4. As the depth of cut becomes smaller, (particularly when the ratio of depth of cut to tool radius becomes \( \sim 0.1 \) or less), the material in the cutting zone will experience a hydrostatic pressure field that is not accounted for in the conventional metal cutting theory. Utilization of strain gradient plasticity may also be appropriate for the small depth of cut used in the experiment.

5. For the conical indenter with included angle 90° and 5 \( \mu \)m nose radius, oblique cutting theory may be more appropriate at 1–30 \( \mu \)m depth of cut.

Work is currently in progress to develop a MRR prediction model for the CMP process based on the concept of material detachment due to scratch intersection.

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