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Simulation of chemical mechanical planarization of copper with molecular dynamics

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With an aim to understanding the fundamental mechanisms underlying chemical mechanical planarization (CMP) of copper, we simulate the nanoscale polishing of a copper surface with molecular dynamics utilizing the embedded atom method. Mechanical abrasion produces rough planarized surfaces with a large chip in front of the abrasive particle, and dislocations in the bulk of the crystal. The addition of chemical dissolution leads to very smooth planarized copper surfaces and considerably smaller frictional forces that prevent the formation of bulk dislocations. This is a first step towards understanding the interplay between mechanistic material abrasion and chemical dissolution in chemical mechanical planarization of copper interconnects. © 2002 American Institute of Physics. [DOI: 10.1063/1.1505113]

Chemical mechanical planarization (CMP) is a critical process in the manufacturing of integrated circuits, multi-level copper interconnects,^{1,2} and synthesis of nanoscale systems such as photonic crystals.³ CMP allows a patterned surface to be completely planarized so that an entirely different metallization pattern can be then fabricated on it, a key requirement in three-dimensional structures. Although the use of CMP technology has advanced tremendously in semiconductor manufacturing, the manufacturing technique has outdistanced itself from the underlying science. The use of CMP in technology focuses on empirical polishing schemes for specific applications with limited understanding of the fundamental interactions involved. A complete atomistic understanding of the physical/chemical mechanisms of CMP is necessary for optimization and development of the CMP process.

CMP involves complex interactions between the polishing substrate, polishing pad, chemical slurry, and abrasive agents.^{1,2} In spite of many components, the fundamental material removal process occurs by the polishing action of an abrasive particle held under pressure by the polishing pad to the wafer surface. It was proposed¹ that CMP of copper has two components: (1) the mechanical abrasion by the abrasive followed by (2) the dissolution of the abraded material from the copper surface by chemical action of the slurry. Here we simulate the basic mechanisms underlying CMP and understand abrasion processes at the atomistic level. Our simula-

tions utilize the well-established embedded atom method (EAM),^{4,5} which has been very successful in modeling the cohesion, elastic properties, and fracture of close-packed bulk metals as well, surface reconstructions and adsorption on metal surfaces. The total energy (U) is the sum of the embedding energy $F(\rho_{h,i})$ to place an atom i in a host electron density $\rho_{h,i}$ at the site of that atom (that incorporates quantum-mechanical contributions to the cohesion of the solid) and a short range pair potential (ϕ), to give

$$U = \sum_i F_i(\rho_{h,i}) + \frac{1}{2} \sum_{i \neq j} \phi_{ij}(R_{ij}). \quad (1)$$

Our workspace is a copper slab with a (001) surface [Fig. 1(a)], with periodic boundary conditions along the y direction and fixed atomic layers on the xz and xy faces. The

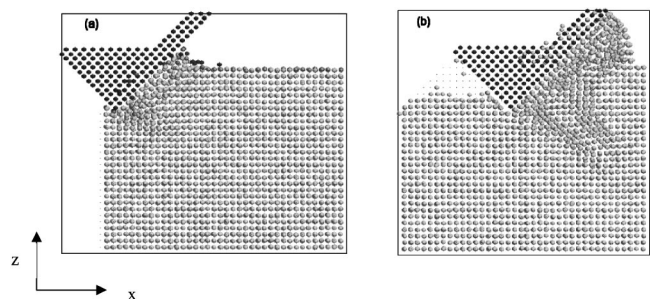


FIG. 1. (a) Early stage of cutting by the abrasive particle on the copper work material at a depth of cut of 1 nm. Mechanical abrasion only is included. (b) cutting of the surface as the abrasive has planarized 3.4 nm of the Cu(001) surface.

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Gear algorithm was used for time integration of the atomic coordinates. The temperature of the lowest eight layers, were controlled to be 300 K by a standard Nose' thermostat so that heat transfers from the surface to the bulk without altering the dynamics at the surface.

The abrasive particle is initially positioned at the left extremity of the work material [Fig. 1(a)] and then displaced rigidly in the 100 direction of the work material. The abrasive is rigid since it is much harder than the copper work piece. The rake angle is -45° . We previously found⁶ that the friction coefficient and frictional forces depend on the shape of the indenter,⁷ but the primary features of planarization do not. Simulations were first performed with a system with a length of 38 rows ($L_x=6.9$ nm) and depth of 30 rows ($L_z=5.4$ nm) containing about 7000 atoms. Simulations were performed on larger systems ($L_x=15.9$ nm or $L_z=10.8$ nm) and found similar results. By using a thin system in the y direction (eight layers, 1.5 nm) we simulate quasi-two-dimensional nanoscale cutting⁶⁻⁹ and reduce computational requirements. This scheme simulates the planarization of a nonuniform copper layer, as in CMP.

We simulate a single polishing event. To understand the interplay between the mechanical and chemical components of CMP, we first simulate surface planarization with the mechanical component only, i.e., without any chemical component. In the second stage described later, we perform a simulation with the chemical dissolution effect incorporated.

The abrasive particle is displaced in small increments (Δx) straight across the sample under the constraint of fixed normal displacement. The normal force on the abrasive varies and depends on the depth of cut. The system evolves with the molecular dynamics algorithm for ~ 50 time steps for each position of the abrasive. For small Δx the simulation approaches a quasicontinuous process. We use a depth of cut of ~ 1 nm typical for CMP and a velocity of cut of 18 m/s. We determined⁶ that at such velocities (2–40 m/s) results are quite similar, the excess heat at the polishing surface dissipates by heat transfer to the bulk, leaving the surface no more than 200 °C above room temperature.

The first set of simulations (Fig. 1) demonstrate the planarization from the mechanistic component of CMP [Figs. 1(a) and 1(b)], which leaves behind a machined surface that is atomically rough. There is considerable disorder and compression of the work material directly ahead of the abrasive. A sizable chip formation (of atomic debris) has occurred ahead of the abrasive in agreement with past simulations of nanocutting.⁶⁻¹⁰ Dislocations are formed at 45° to the polishing direction that traverse from below the abrasive particle into the bulk as the planarization proceeds. The dislocation consists of a pair of extra $\langle 100 \rangle$ rows and would clearly degrade the properties of the copper interconnect.

We next simulate the CMP process by adding a chemical dissolution component. We calculate the potential energy U_i of each atom using the common decomposition of EAM energies

$$U_i = F_i(\rho_{h,i}) + \frac{1}{2} \sum_{j \neq i} \phi_{ij}(R_{ij}). \quad (2)$$

If a surface atom (behind or ahead of the abrasive) has a calculated potential energy U_i higher than a selected thresh-

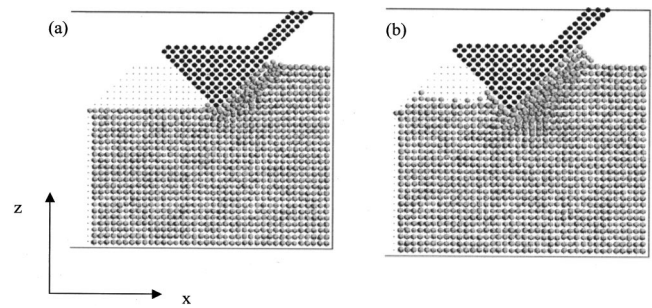


FIG. 2. Planarization of the copper surface when (a) complete chemical dissolution is added with a low threshold energy (-3.5 eV) and (b) when chemical dissolution is incomplete with a higher threshold energy (-2.75 eV).

old energy E , we etch the atom by removing it from the surface and placing it in the solvent—where it no longer interacts with the copper surface. This simple phenomenological algorithm effectively models the expected etching of loosely bound surface atoms and the dissolution of the abraded material into the CMP slurry. By varying the threshold energy we control the rate of dissolution. The existence of the chemical slurry reduces the free energy needed or the threshold energy to separate an atom from the surface. We note that the potential energy U_i is not the energy ΔG to remove the atom from the system, which includes energy contributions from neighbors of the atom removed. Hence the threshold energy is not the chemical potential but related to it. Using the threshold energy criterion provides a workable algorithm for the chemical dissolution.

We performed molecular dynamics of CMP on the same system (Fig. 2) with the added chemical dissolution. The chemical component reveals several beneficial features displaying [Fig. 2(a)] a very smooth planarized surface behind the abrasive, with no defects even at the atomic scale. There is no atomic debris (chip) ahead of the abrasive, since the chip atoms are rapidly etched away. The compression and distortion of the work material in front of the abrasive is considerably smaller than the mechanistic case. A major advantage of the chemical dissolution in CMP is that there are

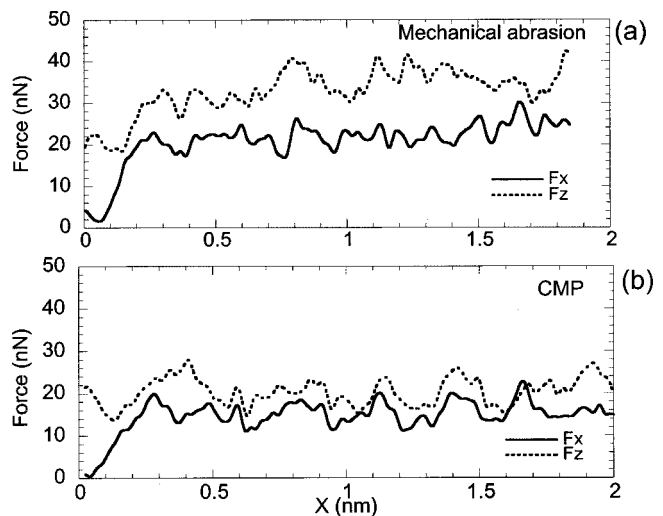


FIG. 3. Cutting force (F_x) and thrust force (F_z) on the abrasive as a function of the planarization distance for (a) simulation with only mechanistic abrasion and (b) simulation with chemical dissolution of atoms.

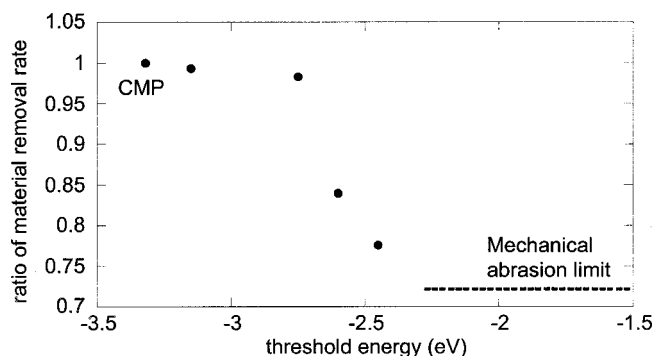


FIG. 4. Calculated material removal rate as a function of the threshold energy for dissolution. The rate is normalized to the value with full chemical dissolution. The CMP and mechanical abrasion limits are shown.

no dislocations in the copper interconnect. Raising the threshold energy and decreasing the etch rate produces a slightly rougher polished surface [Fig. 2(b)] that is still dislocation-free.

The reason for the reduced dislocations can be seen in the variation of the cutting force (F_x) and the thrust/normal force (F_z) on the abrasive particle with planarization distance (Fig. 3), where the coefficient of friction $\mu = F_x/F_z$. For the mechanistic case $\mu = 0.63$ ($F_x = 20.8$ nN, $F_z = 32.9$ nN). With chemical etching both force components are reduced by 40%–50% (14.9 and 20.0 nN) due to the absence of the chip in front of the abrasive. The friction coefficient $\mu = 0.75$ is close to that in the mechanistic case. The smaller forces prevent the generation of dislocations in the copper. The randomness (Fig. 3) arises from the variation of forces generated by the disordered layer in front of the abrasive.

The material removal rate in CMP simulations is more than 40% higher than for abrasion and decreases sharply when the threshold energy is higher than surface atom energies (Fig. 4). Without the chemical effect (Fig. 1), the polishing depth is less than the abrasive depth and some abraded

material falls back on the polished portion of the surface. In this regime the material removal rate is controlled by the chemical dissolution rate, and not the polishing speed as observed experimentally.¹ Alternatively, when chemical dissolution is employed, the polishing depth is the abrasive depth [Fig. 2(a)], and there is no material fallback on the planarized surface. The material removal rate is controlled by the polishing speed in experiment¹ and simulation.

In conclusion we have simulated the fundamental atomic processes involved in the CMP of copper, and observed a rich interplay between the mechanistic and chemical components of CMP. A high level of chemical dissolution in CMP is vital to planarization, increasing the material removal rate, and generating a dislocation free-copper surface.

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