

# Strength of Nanoscale Copper Connection Under Shear

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## ABSTRACT

Strength and shear modulus of several polycrystalline copper systems were calculated with the molecular dynamics method and effective-medium potential. Grain size varied between 2–10nm and systems were sheared beyond the yield point at room temperature. An inverse Hall-Petch behavior was seen: the strength decreased with decreasing grain size. Similar behavior was seen for the shear modulus. These were caused by the grain boundaries, which allow sliding and have low elastic constants. Comparison with tensile strength from another simulation shows that the Von Mises failure criterion holds quite well even at these length scales.

To further study the properties of interconnections, copper-tantalum interface was studied with an embedded atom alloy model. Preliminary results show that the properties of the interface are very sensitive to its microstructure and failure may occur there.

**Keywords:** Copper, nanocrystals, molecular dynamics, interface, tantalum

## 1 INTRODUCTION

Properties and processing of copper have received a lot of interest among electronics community mainly because of its low electrical resistance. Packages used in electronic devices consist of materials that have different coefficients of thermal expansion (CTE) and thermal stress is induced in them when temperature changes, as depicted in Fig. 1(a). As packages become smaller, stress and failure mechanisms can not be accurately analyzed with continuum models, and atomistic molecular dynamics (MD) methods must be used instead, even though the time and size scales that can be studied with MD are very limited. The accuracy of such a simulation crucially depends on the potential. Large scale simulations can not be performed with *ab initio* type potentials, and one must rely on semi-empirical potentials. For many metals, e.g. copper, potentials based on the embedded atom method (EAM) [1] or the effective medium theory (EMT) [2] work well.

In this paper we concentrate on two subjects: the effect of grain size on the shear strength of small scale copper at room temperature (300K) and the strength

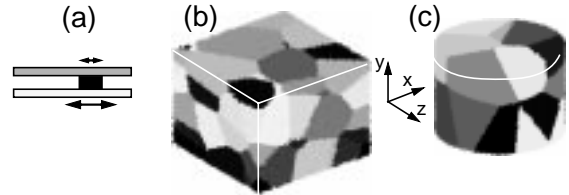


Figure 1: (a) When temperature changes shear strain is induced in an interconnection between two parts with different CTEs. Polycrystalline copper system with periodic (b) and free (c) boundaries. Crystal orientations for each grain are randomly selected.

of a copper-tantalum interface. As a means MD with either EMT or EAM potential is used.

Nanocrystalline copper under tensile stress has been studied by Schiøtz *et al.* [3]–[5]. They studied tensile strength of polycrystalline copper at a very low temperature and later extended the simulations to higher temperatures and various strain rates. However, the loading mode was always tensile even though shear is much more interesting from the interconnection point of view. In addition, Van Swygenhoven *et al.* [6] studied nanocrystalline copper when they compared its properties to nickel, but also they studied only tensile loading.

Apart from polycrystalline structure, strength of a copper connection is affected by the interface between the copper connection and the component. As copper diffuses easily into silicon, a barrier layer is needed. It seems that tantalum is used most often, even if many other metals are also suitable [7]. Often the interfaces and other disordered parts of the system are the weakest spots [8] and therefore their role needs to be analyzed.

## 2 MODEL

In case of polycrystalline copper the interaction between copper atoms is described by the effective-medium theory (EMT) [2]. This potential was used by Schiøtz *et al.* [3]–[5], and therefore the comparison can easily be made. However, alloys are much more easily described in context of embedded-atom method, and it is used in the interface calculations. The many atom nature of metallic cohesion is crucial in describing the mechanical properties of metals, which is a point where these many atom potentials have a clear advantage over the classi-

cal pair potentials. The central idea in both potentials is to embed the positive ion into electron gas, which is formed by the free electrons of the metal atoms.

These potentials work best near equilibrium, but far from equilibrium problems may rise due to the finite range and the way the potentials are cut [9]. Here we cut the potentials smoothly between third and fourth nearest neighbors of ideal copper. The EMT model can accurately reproduce many properties of copper, such as the stacking-fault energy and elastic constants, cf. [9] and references therein for details. In case of EAM, the potential is cut quite rapidly, since the cut-off distance must be less than 3rd neighbor distance in ideal tantalum. For the EAM potentials we refer to [10] and [11]. However, both the potentials were cut as proposed in [11]. Thus, some of the properties of the model copper are slightly different from [10]. The elastic constants ( $T=0\text{K}$  and  $T=300\text{K}$ ), intrinsic stacking-fault energy, CTE, and minimum energy configuration were compared with available experimental data, and the results were very good.

### 3 RESULTS AND DISCUSSION

The shear strength was studied by shearing the system beyond the yield point. This was done by fixing the locations of the atoms at the topmost and bottommost boundaries and by moving them in the x direction with a slow strain rate, about  $100\%/ns$  unless otherwise specified. This strain rate is in between the limits proposed for copper in [12] and in a previous study [13] this was found to be sufficiently low a rate to study system strength.

During the shear test temperature was controlled with a Nosé-Hoover thermostat that was smoothly in connection with the boundaries of the system as discussed in [14]. Thus the dynamics in the middle part of the system were purely Newtonian and based on the potential.

#### 3.1 Polycrystals

Both periodic and free boundary conditions were used, as shown in Figs. 1(b) and (c), respectively. The height of the system was  $13\text{nm}$  and the cross sectional area (circular or square with free or periodic boundaries, respectively) was  $13\text{nm}^2$ , which totals in approximately  $210\,000$  atoms.

The polycrystalline microstructure was generated by performing the Voronoi partition, as in [3] and [6]. The location and crystal orientation for each grain was selected randomly, though such that two grains were located at least five lattice constants from each other. For each grain, the space closer to that grain than to any other grain was filled with an FCC structure. Initially the system was thermalized to equilibrium at tempera-

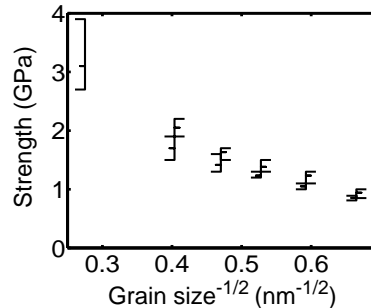


Figure 2: Strength of polycrystalline copper as function of inverse square root of grain size. The vertical lines indicate the minimum, maximum and average values taken from six simulations. The lines pointing to left (right) correspond to free (periodic) boundaries.

ture  $T = 300\text{K}$  to allow unfavorable configurations near grain boundaries to relax.

The volume of the system was about  $\Omega = 2\,300(\text{nm})^3$  and it was divided into  $N_G=1, 10, 25, 50, 100,$  or  $200$  grains. This corresponds to grain sizes  $l_G=13, 6.1, 4.5, 3.6, 2.8, 2.3,$  and  $1.8\text{nm}$ , respectively, where  $l_G=(\Omega/N_G)^{1/3}$  is a measure of average grain size. In practice copper systems with grain size down to  $4\text{nm}$  can be produced by means of inert gas condensation [15]. Other methods to produce fine grained metals are discussed e.g. in [16].

The shear modulus and strength of the systems were studied. As a measure of strength, the maximum stress is used. In addition to maximum stress, Schiøtz *et al.* [3] calculated the yield stress from the point where the stress as function of strain deviated from linearity. However, the stress behavior of room temperature EMT copper is nonlinear already before any plastic deformation takes place and deviations due to finite temperature make this approach very complicated. Therefore the maximum stress is used to characterize strength. For a given grain size, six systems were studied (locations and orientations of grains were selected randomly) with both periodic and free boundaries.

Fig. 2 shows the strength of the system as function of inverse square root of grain size. It is seen that the strength decreases almost linearly as function of  $l_G^{-1/2}$ . Thus the strength of copper under shear behaves in a similar way to the strength under tension [3]. In addition, the quantitative results are quite close after the application of the Von Mises failure criterion [17]. As an example, Schiøtz *et al.* [4], [5] obtained the tensile strength  $1.9\text{GPa}$  for the grain size  $l_G=5.2\text{nm}$ . In our systems this would correspond to about 20 grains, and thus the value they obtained is about one quarter lower than what might be expected ( $\sqrt{3}\times 1.6\text{GPa}=2.7\text{GPa}$ , cf. Fig. 3). However, their strain rate was only  $50\%$  in ns. To find out whether the above discrepancy is due to different strain rate we tested the dependence of strength on strain rate and studied systems with  $N_G=10, 25,$  and

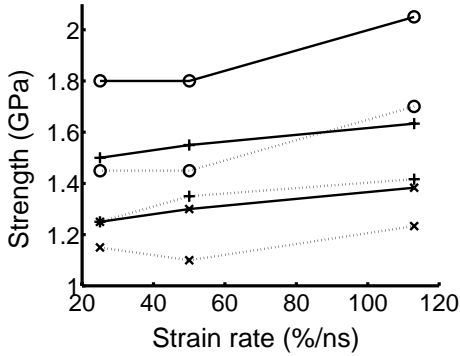


Figure 3: Strength of polycrystalline copper as function of strain rate and grain size. The system with periodic (solid line) or free (dotted line) boundaries consist of 10 (o), 25 (+) or 50 (x) grains.

50. Shown in Fig. 3 is the strength as function of grain size and strain rate. It is seen that the strength is not heavily dependent on strain rate, and the strain rate can not explain the difference of the results. Thus it is seen that above failure criterion can be used only approximately to relate the tensile and shear strengths of the systems. However, it is important to realize the weakening of the system with decreasing grain size, even under shear deformation.

In addition to strength, the modulus of the system decreases when the grain size decreases. The dependence was nearly linear as function of  $l_G^{-1}$  and the shear modulus of systems with  $l_G=1.8-6.1$ nm, ranged between 18–38GPa or 25–45GPa with free and periodic boundaries, respectively. A low value for the Young’s modulus of nanocrystalline copper has been experimentally measured [15], 36–45GPa for grain sizes 50nm or 25nm as compared to 130GPa for large grained copper. Following linear elasticity this would imply a shear modulus of 13–17GPa for nanocrystalline copper. Thus the values of the shear moduli are in good agreement.

The modulus decreases because the modulus of the grain boundaries has been shown to be much smaller than that of bulk copper [3], [14], [18], particularly the shear modulus parallel to grain boundaries seems to decrease very much [19]. Furthermore, in a system with small grains, the grain boundaries occupy a large fraction of the total volume and thus have a strong contribution to the properties of the whole system. The difference of the modulus of the grain boundary as compared to the modulus of the bulk may rise from nonlinear elastic behavior and the fact, that the grain boundaries themselves are strained as compared to bulk [18], [20].

After the yield point most plastic deformation is accumulated at the grain boundaries. One way to characterize the deformation is to study the rotation of the grains as a function of external strain [5]. This is shown in Fig. 4. For each grain the rotation of the basis vec-

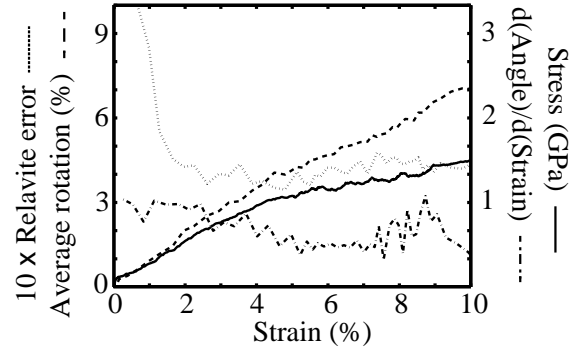


Figure 4: Average rotation of grains around z-axis (dashed), its numerical slope (dash-dot), relative error (standard deviation per average, dotted), and shear stress (solid line) as function of shear strain in a system with free boundaries. Initially there is almost a one to one correspondence between the angle and strain. When the system yields, further deformation results in smaller grain rotations than in the elastic case.

tors of the lattice, around z and x-axis, is calculated as function of external strain, and the rotation around z axis is shown. Initially the average rotation equals the strain, as in the elastic case should be. The slope is very close to one for strains less than about 2%, as seen from Fig. 4. Later when the system starts to plastically deform, the slope decreases to about one third, i.e. some of the total deformation takes place without grain rotation. This bears evidence of grain boundary sliding in the systems.

### 3.2 Interface

The copper-tantalum interface was generated by depositing copper atoms on an ideal BCC tantalum block at  $T=300$ K, as depicted in Fig. 5(a). The initial tantalum system consisted of 40000 atoms, and 60000 copper atoms were deposited on it in 40ps. The system formed in this way is a cube with an edge of about 110Å. After the system was generated, it was thermalized closer to equilibrium for another 40ps. Diffusion of Ta into Cu or vice versa was minimal, even though the heat of formation of the binary alloy is negative. Three different systems were generated: The plane of the interface corresponded to the (100), (110), or (111) plane of the tantalum system. The systems were sheared, as shown in Fig. 5(b) to find out where the failure starts, and is the system significantly weaker than a pure Cu system.

As the elastic constants of Ta are much larger than those of Cu, the strain in Ta is much smaller than in Cu. Furthermore, since the yield stress of ideal BCC tantalum with the above crystal orientations and at  $T=300$ K ranges between 3.6–16GPa, failure did not occur in Ta. The location of failure depended on the system. It occurred in pure copper in two of the systems (the plane of the interface was (100) and (111), stress about 500MPa),

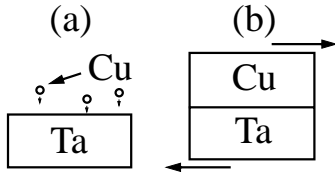


Figure 5: (a) Deposition of copper atoms on a tantalum sheet at room temperature, with periodic boundaries. (b) Shear test of the interface.

and at the interface in one (interface (110), stress about 250MPa). Cohesion at the interface seems to explain these differences. In the system that failed at the interface the electron density for copper atoms next to the interface was significantly lower than in other systems. Thus the cohesive forces were smaller, and sliding along the interface took place. Different cohesive forces are due to different microstructures. Thus it is seen that the crystal orientations at the boundaries have significant effect on the strength of the interface.

#### 4 SUMMARY

We have studied the effects of polycrystalline microstructure on the strength of nanoscale copper systems under shear deformation. The results are very similar to those observed by Schiøtz *et al.* despite the different loading mode. The strength decreased as the grain size decreased. This is qualitatively in agreement with tensile simulations. Furthermore the value of strength was in quite good agreement when the factor  $\sqrt{3}$  due to the Von Mises failure criterion was applied. Most of plastic deformation took place in the form of grain boundary sliding. The interface between copper and tantalum may be the weakest spot in the system. However, the strength of the interface depends heavily on the cohesive forces which further depend on the microstructure of the interface.

It seems that the mechanical properties, particularly the strength, of a nanoscale copper connection depend crucially on the microstructure and interface. While the interface can be the weakest spot, the strength of the connection itself decreases as the grain size decreases. However, when optimizing the strength of such nanoscale copper systems, one has to bear in mind that the properties of crystals that consist of only a few crystallites are heavily dependent on the crystal orientations of the crystallites and loading. These issues affect also the strength of a copper-tantalum interface and need therefore to be studied in more detail in the future.

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