# Molecular Dynamics Study of Thermally Induced Shear Strain in Nanoscale Copper

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## ABSTRACT

We study the effects of thermally induced shear strain and stress in several nanoscale copper systems consisting of about 200k atoms with the effective-medium theory and molecular dynamics method. Both edge and screw dislocations are seen to initiate at the free boundaries on the {111} slip plane. In most cases dislocations are slower than the speed of sound, but a transition to supersonic edge dislocations was observed. In some cases dislocations initiated at the compressive side of the system rather than at the tensile side. This was proposed to be caused by the dependence of the stacking fault energy on the state of strain. The results show that initially the stress is concentrated in the corners of the system, and later, when the structure has been plastically deformed, high stress regions are found in the center of the system. The minimum stress and strain at which plastic deformation occurred were 1.2GPa and 4.6%.

***Keywords***: Copper, molecular dynamics, dislocation, interatomic potential, stacking fault energy

## INTRODUCTION

Since 1995 when IBM proposed [8] that copper can be used in electrical interconnections, its properties have received a lot of interest in the electronics community, mainly because of its low electrical resistance. Such electrical structures consist of materials that have different coefficients of thermal expansion (CTE) and thermal stress is induced in them when temperature changes. In very small systems and in order to understand deformation mechanisms, atomistic effects (e.g. structure) has to be taken into account correctly. At the microscopic length scale the molecular dynamics (MD) method [1] takes correctly into account these effects, when the potential is chosen correctly. For copper the potentials based on the embedded atom method (EAM) [2] or on the effective-medium theory (EMT) [9] work well and can be considered as state of the art potentials for metals. However, the time and size scales that can be studied with the MD method are very limited. Typical time scales are measured in ps and size scales in Å. Parallel computing methods allow simulations of much larger systems [14], but not many scientist have access such huge computing resources, and the simulations become extremely time consuming, when the interesting parameter space is large (structure, temperature, strain rate, etc.) In previous studies [5], [6] we have seen, that the results for copper obtained with the EMT potential are very good for systems of more than $10^5$ atoms.

## POTENTIAL

In these simulations the interaction between copper atoms is described by the effective-medium theory (EMT) [9], which is an approximate method for calculating the total energy of a system of metal atoms from their positions. The many-atom nature of metallic cohesion is crucial in describing the mechanical properties of metals, which is the point where many-atom potentials have a clear advantage over the classical pair potentials. Compared to other many-atom potentials for metals, EMT has the strongest *ab initio* nature since, in principle, all the parameters needed in the total-energy expression can be calculated using the jellium model. Because of the functional form of the potential — although the calculations are performed for the specific case of copper — we expect that the qualitative conclusions will remain valid for a wide set of pure fcc-metals. For the functional form and other details of the potential we refer to [3], [4].

## LOADING AND TEMPERATURE

One case, in which the copper system becomes deformed due to a global mismatch between the CTEs is bumping. As both copper interconnections and flip chip technologies become more popular, it is likely that also the bumps joining the chip and the board (PCB) are in part made of copper. When this small copper bump joins two materials that have different CTEs, shear strain is induced in the system. Loading is imposed by using fixed y boundaries, cf. Fig. 1. Three crystal orientations were studied, the (y,x) crystal orientations being ([010],[100]), ([011],[01$\bar{1}$]), ([111],[2$\bar{1}\bar{1}$]) and $\vec{z} = \vec{x} \times \vec{y}$. The height of the cylindrical copper bump was 130Å and the diameter of its cross section was 150Å making the size of the system about 200k atoms. Because this size is twice the limit we proposed in [5], we expect the simulations to predict the deformation mechanisms

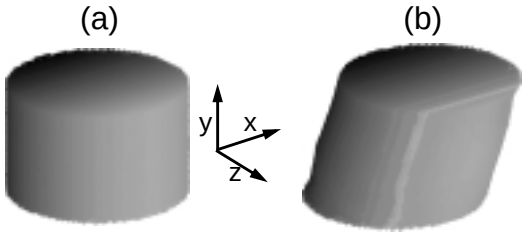


Figure 1: System at rest (a) and under shear strain (b) induced by the CTE mismatch between the chip and the board.

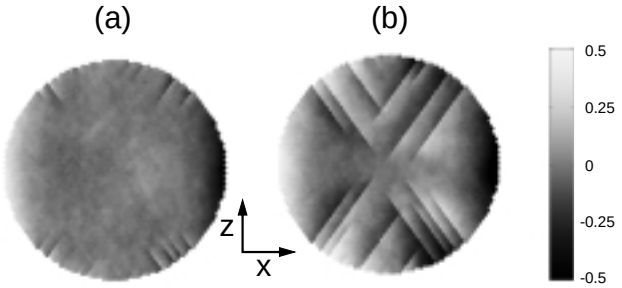


Figure 2: Slip in the y direction at the center of the system. Due to symmetry the results are similar at all heights. Shading indicates the y component of the slip for for each atom (scale on right in lattice constants). Slipping produces a (whole) screw dislocation with the Burgers vector of the form a/2[011]. The time difference between the figures is 1.6ps.

in the atom scale correctly. Initially the system was thermalized to equilibrium at temperature $T = 456$K. Thereafter the temperature was decreased to $T = 233$K in time $t_0$. When dislocation initiation was studied, two strain rates were used: $t_0 = 200$ps and $t_0 = 20$ps. We studied also cyclic strain, where the ramp and hold times were $t_0 = 20$ps and $t_0 = 10$ps. It is noted that even though the relaxation period (10ps) is very short, an elastic wave can propagate back and forth the system approximately two times during it. The internal temperature of the system was controlled with a Nosé-Hoover thermostat [11]. For the above temperatures and system size, reasonable values for the distance from neutral point (DNP) and CTE mismatch gave the maximum shear strain 30%, cf. Fig. 1.

## DISLOCATION FORMATION

It is well known (cf. e.g. [7]) that in an fcc structure slipping most often occurs along a {111} plane. Thus the mutual orientation of this plane and the direction of strain determines how a dislocation initiates in the defect-free system. We studied three different geometries as described above, and the results are described below.

First we studied the case y=[011], x=[01$\bar{1}$], z=[100] with the strain rate 30% in 20ps. In this case the dislocations initiated at the free boundaries and slipping occurred along the ±z±x planes. The Burgers vector was parallel to the direction of y, which was also the direction of the dislocation line. Thus the dislocation was a screw dislocation, cf. Fig. 2. It can be seen that the speed of these screw dislocations in bulk copper is approximately 2500m/s, which is slightly less than the speed transverse shear waves in copper, 2900m/s [6]. This is in accordance with dislocation theory [7], since in case of screw dislocations the speed of transverse shear waves is the theoretical limit for the speed of dislocations. With the lower strain rate (30% in 200ps) the above results did not change either qualitatively or quantitatively. Thus it seems that dislocation initiation and propagation are independent of strain rate at least for time scales short enough to neglect creep and long enough with respect to the speed of sound and the system size. The critical shear stress at which the dislocations initiated was 1.5GPa and 1.3GPa with the low and high strain rates, respectively and the corresponding shear strains were 9.8% and 8.6%. Also these values indicate, that the behavior is not heavily dependent on the strain rate.

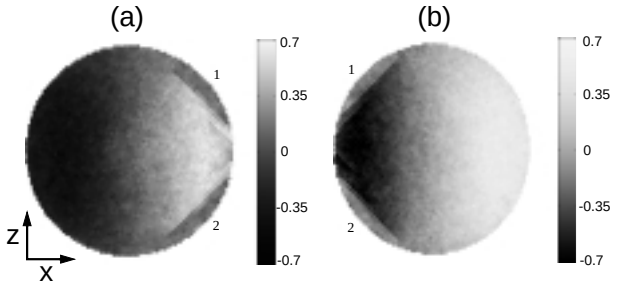


Figure 3: Slip in the y direction at the bottom (a) and top (b) of the system. Shading indicates the y component of $\vec{d}$ for each atom (scale on right in lattice constants). Slipping produces partial edge dislocations with the Burgers vectors of the form a/6[112]. Such dislocations occur on subsequent {111} planes resulting in a twin crystal structure.

Next we studied the case, where y=[010], x=[100] and z=[001], using the strain rate 30% in 20ps. The {111} planes were of the form ±x±y±z and dislocations initiated at the free boundaries near both the top and the bottom boundaries (cf. Fig. 3). These dislocation were Shockley partials, which occurred on subsequent {111} planes, creating a twin crystal structure. When the stacking fault energy (SFE) of copper was studied (cf. below), it was seen that also in this model the SFE is to proportional to the number of {111} planes in the hcp structure, at least to a good approximation, cf. [12]. Thus the energy of an intrinsic SF and an extrinsic SF are equal and twice the energy of a twin fault. Therefore the twin structure is preferred compared to structures with several stacking faults occurring not exactly on subsequent planes.

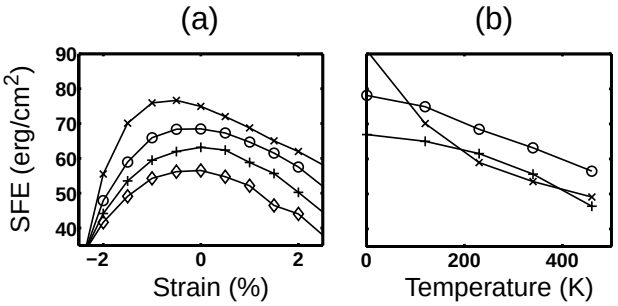


Figure 4: (a) Stacking fault energy as function of uniform strain at temperatures 120K(x), 230K(o), 340K(+) and 460K($\diamond$). SFE as function of temperature for strains -1.5% (x, i.e. 1.5% compression),0%(o) and 1.5%(+).

Many finite-element calculations (cf. e.g. [10]) in a solder joint under similar loading show, that most plastic deformation occurs near the boundaries, where the state of stress is tension (i.e. top, large x and bottom, small x). However, in case of copper, dislocations initiated at locations, where the stress was *compressive* rather than tensile (cf. Fig. 3). This can be explained with the SFE. In Fig. 4 we show the SFE as a function of external strain and temperature calculated with the present model. It is noted that the SFE refers to an intrinsic SF. From Fig.4(a) it is seen that for large strains the SFE is smaller under compression than under tension. Thus less energy is needed for SF formation under compression than under tension, explaining dislocation initiation at the compressive side. Furthermore, from Fig. 4 it is seen that the temperature dependence of SFE in a stress less system agrees extremely well with experimental data by Shetty [13]. Specifically he found that the SFE, $\gamma$, depends on temperature (T in K) as $\gamma/\gamma_{300} = 1.2 - bT$, where $b = 828 \times 10^{-6}/K$ and $\gamma_{300}$ is the SFE at 300K. From our calculations $b = 744 \times 10^{-6}/K$, which is slightly less. However the SFE we obtained at T=0K (79ergs/cm$^2$) is somewhat more than the experimental value (30-80ergs/cm$^2$ cf. e.g. ref. 41 in [4] and [12]), which is one reason for too small a value for $b$.

When the strain rate was decreased by a factor of ten the deformation mechanism did not change from that described above. However, strain rate affected the dislocation velocities. In case of edge dislocations, the limiting speed for dislocations is not the transverse sound speed. For slowly accelerating edge dislocations the Rayleigh speed should be an upper limit, but for very rapid loadings even this limit can be exceeded [7]. This transition from super-sonic to sub-sonic dislocation was seen as the strain rate was decreased from 30% in 20ps to 30% in 200ps, i.e. loading was changed from rapid, impact-type loading to slow loading. For the higher and slower strain rates the dislocation velocities were 3700m/s and 1200m/s, respectively. Clearly the first is above and the latter below the Rayleigh speed in copper, $c_R = 2020$m/s. The critical shear stress was 1.6GPa and 2.0Gpa for slow and rapid deformation, respectively and the corresponding shear strains were 4.6% and 6.8%. Thus, in terms of strain, the system failed most easily in this direction. When the vertical direction was set y=[111], and the other orientations x=$[2\bar{1}\bar{1}]$ and z=$[01\bar{1}]$, it was evident, that the slip should form parallel to x direction. However, just before the slip started to form, a dislocation with the Burgers vector a/2$[01\bar{1}]$ was seen on a (133) plane in the center of the system. Slipping in the x direction occurred at the point of maximum stress, which was 2.5GPa and 3.0GPa in the slow and fast deformation test. The partial dislocations propagated in the x direction with the velocities 3500m/s and 1300m/s for the fast and slow deformation. Even though the stress, at which these dislocations occurred, was about 50% greater than in systems with the previous geometry, the velocities of the dislocations were approximately equal. This bears evidence, that the velocity of the Shockley partials is not dependent on the state of stress, as long as the stress is large enough for dislocation initiation.

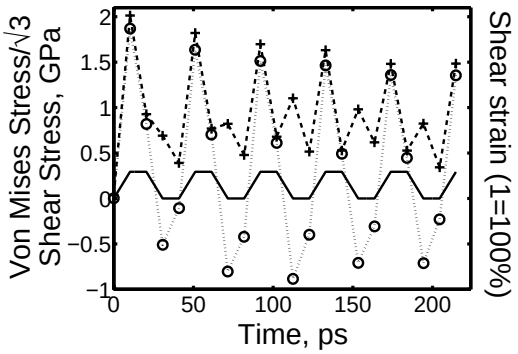


Figure 5: Shear strain (solid line), shear stress (dotted line, o) and the Von Mises stress divided by $\sqrt{3}$ (dashed line, +) as functions of time. Zero strain corresponds to temperature $T = 456$K and 30% strain to $T = 233$K, results are for the case $y = [011]$.

## STRESS CONCENTRATION UNDER OSCILLATORY LOADING

In addition to dislocation initiation, we studied what happens, when the temperature and strain oscillates. In Fig. 5 we show the strain and the shear stress as function of time. The stress needed for deformation seems to decrease as function of time. In addition, initially the (absolute value of) stress needed to move the boundaries to their initial locations seems to increase. However, after three thermal cycles these stresses decrease as well. Thus it seems, that the long term behavior of the system becomes detectable only after three initial thermal cycles. The number of thermal cycles, after which the range of stress started to decrease depended on the ge-

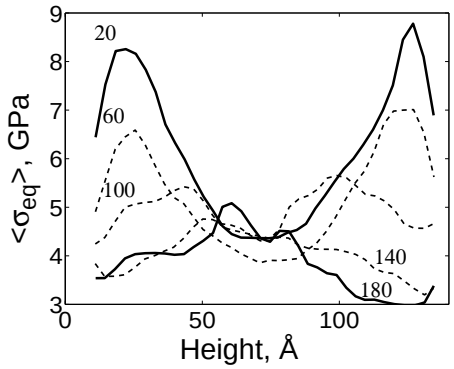


Figure 6: Average Von Mises stress as function of height ($y = [011]$) after loading and relaxing the system. The corresponding time in ps is depicted above each curve.

ometry, but was six at most.

Initially the stress seemed to concentrate to the corners of the system as depicted in Fig. 6. However, the plastic deformations affect the stress distribution such that the high stress-regions move to the center of the system. This is depicted in Fig. 6, where we show the distribution of the Von Mises stress as function of time and height. Interestingly, the distribution has two peaks for times 20, 60 and 100ps, but only one peak thereafter. When compared with the shear stress in Fig. 5 it is seen that the minimum shear stress starts to increase after $t = 140$ps, i.e. when the stress in Fig. 6 has only one peak.

## SUMMARY

We have studied dislocation initiation and propagation in nanometer-scale copper systems. Dislocations initiated because of an external shear loading, that was induced in the system due to a mismatch between the thermal coefficients of expansion of the materials surrounding the copper bump. In addition to system geometry, strain rate was also a parameter, whose role we analyzed. In all cases the dislocations propagated along the well known {111} planes. Both screw and edge dislocations were seen, depending on the mutual orientation of loading and the lattice. The edge dislocations were Shockley partials in both cases. Crystal twinning was also seen. It turned out that qualitatively the results were not affected by the the strain rate. However, quantitatively the results depended on the strain rate. The most noteworthy strain rate dependent phenomenon, which is predicted also in the context of dislocation theory, was the transition from super-sonic to sub-sonic edge dislocations. This occurred, when the strain rate was decreased from rapid to slow loading. The minimum shear stress, at which the dislocations initiated was as high as 1.2GPa. The minimum shear strain was 4.6%, which occurred in a different system, due to the different shear modulus. Although polycrystalline copper is somewhat weaker due to grain boundary sliding, these values can guide the development of Cu-bumps. In the oscillating load test stress initially concentrated to the corners of the system. However, later the stress seemed to concentrate to the center of the system somewhat in contrast to the other studies. On the basis of the studies we proposed that in a small copper system under oscillating shearing, the long term behavior becomes detectable already after a few, six at most, first cycles.

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