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Deformation Behavior of FCC Crystalline Metallic Nanowires Under High Strain Rates

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ABSTRACT

We used molecular dynamics (MD) methods to study the deformation behavior of metallic alloy crystal nanowires of pure Cu, NiCu alloy and NiAu alloy, under high rates of uniaxial tensile strain, ranging from $5 \cdot 10^8/s$ to $5 \cdot 10^{10}/s$. These nanowires are just about 2 nm thick and hence cannot sustain dislocations, instead we find that deformation proceeds through twinning and coherent slipping mechanisms. NiAu has a 13% size mismatch whereas NiCu only 2.5%. As a result the critical strain rate at which the "nanowire crystals" flow like a "liquid" is 100 times smaller for NiAu. We also calculated the elastic constants at each strain state for all strain rates to identify the relation between mechanical "shear" instability and deformation process.

INTRODUCTION

From mechanical tests and structure analyses such deformation mechanisms as, dislocations[1][2], twinning[3][4], and grain boundary sliding[5]. have been proposed and verified in various systems. The two major and competitive deformation models in single crystal are slip and twinning, increases in strain rate or decreases in temperature tend to favor twinning over slip. Deformation twins are more prominent in bcc and hcp metals than in fcc, because the five independent slip systems required for general deformation may not be satisfied in bcc or hcp. Indeed twins have been observed. in fcc metals exposed to large strain rates (such as in shock waves [6]), and/or low temperature [7]. Unfortunately experiments under these conditions, tend to have many factors all playing a role simultaneously. For instance, experiments at very high strain rates lead to shear localization arising from adiabatic heat dissipation and localized thermal softening.

On the other hand , molecular dynamics (MD) simulations can isolate the direct effect of strain at various strain rates from those due to heat dissipation and the concomitant temperature increase by controlling the temperature and the strain rate. Keeping the temperature constant and can then be used to analyze the detailed mechanisms of the deformations.

SIMULATION METHODS

The periodic unit cell for the MD simulations consisted of $5 \cdot 5 \cdot 10$ fcc cubic cells ($1.78nm \cdot 1.78nm \cdot 3.56nm$ for NiCu) with 1000 atoms. We started with an fcc single crystal and

equilibrated at 300K for 100 psec. For the alloys NiCu(50%) and NiAu(50%) we assumed a random fcc structure. We used 1-D periodic boundary condition along the $\langle 001 \rangle$ crystallographic direction [8], but a finite wire (about 2nm thick) in the x and y directions. The tensile strain, ϵ_{33} , was applied in the z direction to these infinite nanowires. To maintain the specified strain rate, the tensile strain along the $\langle 001 \rangle$ direction was increased by 0.5% at a time interval determined by the strain rate. To avoid the generation of stress wave, the strain was applied uniformly to all layers of atoms, which were then allowed to relax in the MD under isokinetic conditions (kinetic energy is kept constant). This isolates effects of adiabatic heat dissipation and thermal softening. At each strain state, we evaluate the stress, the elastic constants (the Born term contribution). Although our nanowire is periodic in only one dimension, we use the true atomic volume to calculate intensive variables.[9]

To obtain accurate properties for the simulations, we use the simulation is a quantum Suttner-Chen (Q-SC) many body force field.[10][11]. Q-SC leads to accurate values for the mechanical, thermodynamic, viscosity, and surface properties (for such as pure metals such as Cu and Ni and for alloys such as CuNi and NiAu). We observed Ni and NiCu lead to similar behavior but NiAu behaves very differently due to the large atomic radii difference.

RESULTS and DISCUSSION

Figure 1 shows snapshots at 100% strain for different strain rates, and figure 2 displays the stress (σ_{33}) - strain (ϵ_{33}) curve for NiCu at T=300K for each strain rate. The stress-strain relation is linear at small strain, and the yield stress increases as the strain rate increases

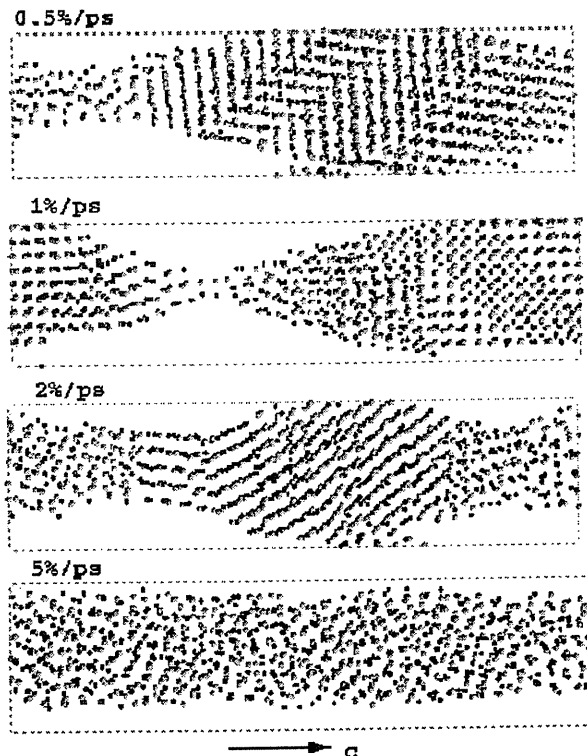


Figure-1, Snapshots of NiCu nanowire at 100% strain deformed at strain rates of

- a. 0.05%/ps shows twinning and local melting in bulk
- b. 1%/ps shows smaller fcc grains
- c. 2%/ps shows extensive disorder
- d. 5%/ps shows full amorphization to glass

At low strain rates, 0.05%/ps and 0.5%/ps, the stress drops in a repeating loading/plastic

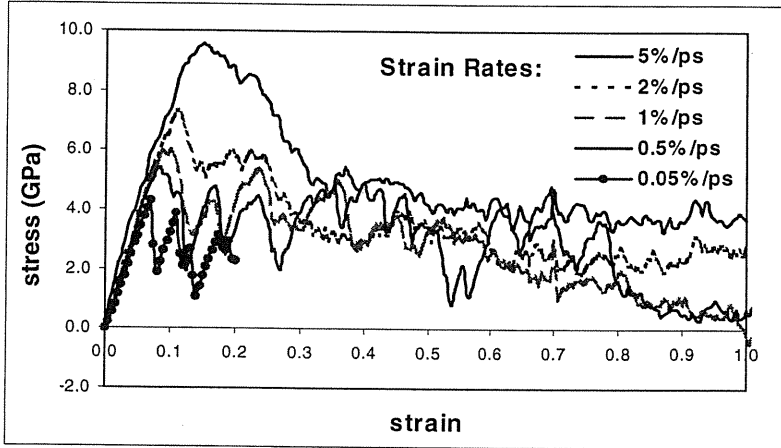


Figure-2. Stress strain curve for NiCu at different strain rates

flow cycle after passing the elastic limit. From analyzing the structures, we have been able to identify these events as coherent shearing, and the twinning formed during the shearing events. The stress drop is due to twin deformation. During the next increase of the stress, the Young's Modulus remains almost the same. Multiple coherent shearing continue to take place as tensile stress increases, but eventually necking begins around 80% strain for strain rates of 0.5%/ps and 1%/ps, and sample becomes disordered around the necking part. Eventually the stress concentration at the neck causes failure, with the stress dropping to zero. After fracture additional increments in strain cannot cause any increase in stress, however the melted neck relaxes back to fcc crystalline packing in the absence of the stress field.

But when the strain rate is increased to 5%/ps we see quite different behavior, At 5%/ps strain rate, no coherent shear bands and twins are formed within the specimen. Instead, the specimen transforms homogeneously into a disordered amorphous state, and undergoes uniform flow without twinning or necking. We reported this strain induced amorphization by analyzing the radial distribution function and elastic constants in an early work.[12]

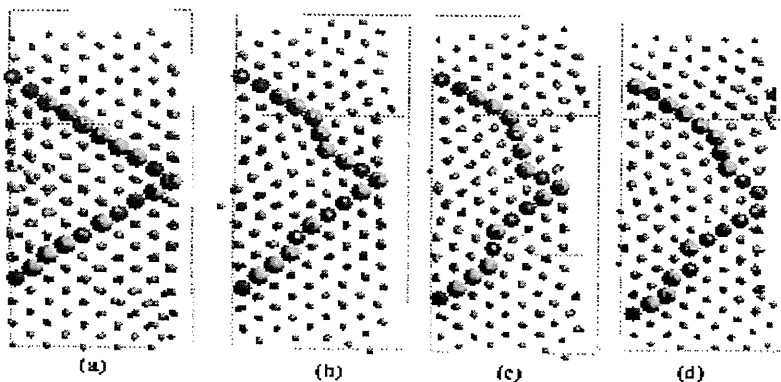


Figure-3 snapshots for NiCu during tensile tests.

- (a) strain rate = 0.05%/ps
strain = 7% before yielding
- (b) strain rate = 0.05%/ps
strain=8%, two twins formed
- (c) strain rate = 0.05%/ps
strain = 14%, twins grow one more layer
- (d) strain rate = 0.5%/ps,
strain = 12.5%/ps,
three twins formed

To study the structural details, we show the $(01\bar{1})$ projection of the structure before and after yielding at strain rate of 0.05%/ps in figure 3. We highlight a group of neighbor atoms on (111) and $(\bar{1}11)$ planes, and keep track of them. The mismatch on (111) planes are obvious in the structure at 8% strain, right after the first load drop. There are two twins formed; one with two $(\bar{1}11)$ layers of atoms, and one only has one (111) layer of atoms. These twins are formed by cooperative shearing, and to return back to the original crystal orientation, there are two stacking faults at each side of the twin. The relative displacements for the atoms across the twin boundary is about $\langle \bar{2}11 \rangle$ on (111) planes, consistent with the well known $(111)[112]$ twin system in fcc metals. The schematic of twinning in fcc metals is given in figure 4, the projection from (220) plane is included to keep the same view as the snapshots shown in figure 3. At a strain state of 14%, the second stress drop finished, and both twins increased by one more (fig3-c). Cottrell and Bilby[13] predicted that the fcc structure would produce only a monolayer stacking fault, and Venables[14] suggested a modified mechanism to allow a continuous growth of twin from a single stacking fault. Our observation agrees with this model.

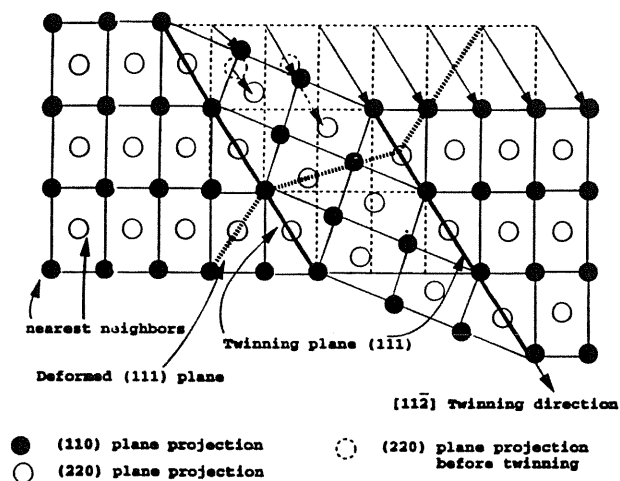


Figure-4, schematic of twinning in fcc metals

The twin deformation causes the stress drop, which in general increases with increasing temperature and the number of stacking faults. We can estimate the energy caused to form four stacking faults (there are four interface for two twins), from the stacking fault energy[15] of Ni (150mJ/m^2) and Cu (80mJ/m^2). We counted the number of atoms of the surface, and calculated the area of the surface (3.29 nm^2 and 4.19 nm^2), then use the average of stacking fault energy for Ni and Cu, 115mJ/m^2 , to obtain the stacking fault energy as $8.602 \times 10^{-19}\text{ J}$. The elastic energy drop during the twinning process is $9.6 \times 10^{-19}\text{ J}$. Thus the system has used the stored elastic energy to form twins. The similar deformation mode has been observed in pure Ni.

Since the system can accumulate more strain energy as the strain rate increases, it is possible that the sample can nucleate more stacking fault for twin growth. The structure of NiCu at 12.5% strain state(right after the first stress drop) under strain rate of 0.5%/ps has show in figure 3-d. Here we observe two independent monolayer stacking faults on the (111) planes. The stress drop at this strain rate is also larger than the drop at 0.05%/ps strain rate.

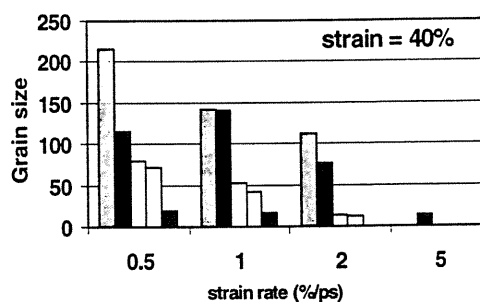


Figure-5, grain size of multi-oriented crystal after twin deformation decreases as strain rate increases.

Figure 1 shows that after the single crystal turned to a multi-oriented crystal by continuous twinning, the grain size at the same strain state but different strain rates are different. We can show qualitatively that the grain size is decreasing as the strain rates increases. We define an atom having 12 nearest neighbors with a ABC packing sequence as a part of a perfect fcc crystal, from it we check the atoms in far nearest neighbors, and stop at the atoms, which lost the fcc nearest neighbors configuration. This method can identify a stacking fault on a twin boundary. Using this method we define the atoms inside the boundary as the grain size. The grain sizes at strain=40% states calculated by this method are given in figure 5. At strain rate 0.5%/ps, we got one grain with 215 atoms and one with 115 atoms, at strain rate 2%/ps, we still have one grain with 112 atoms, while at strain rate 5%/ps, we only found one little cluster with 13 atoms with a fcc structure. The size of grains decreases as the strain rates increases by two reasons, one is more nucleus can form, and the other is to release more stress energy, the deformed nanowire tends to form more twins, as the strain rates increases.

We can propose a deformation mechanism at high strain rates. Here the twin is considered as a unit, it's size decreases as the strain rate gets higher, after a critical strain rate, these units lose their coherent relation, and get smaller than 12, the number of nearest neighbors for fcc, a disordered system emerged. This is the amorphization behavior we observed at 5%/ps strain rate, when system flows like liquid after the transition.

This critical strain rate is a function of temperature and size difference for alloys. As AuNi, which has a large size mismatch, favors the glass formation, thus the critical strain rate to deform like liquid is much lower. We found at strain rate of 0.5%/ps is sufficient to obtain amorphous NiAu. The size mismatch destabilizes the crystalline state with respect to the amorphous state.

CONCLUSIONS

We studied the deformation behavior of Ni, CuNi and NiAu at high strain rate, from 0.05%/ps to 5%/ps. A new deformation mechanism at high strain rate is found. In systems where dislocations cannot be sustained, coherent shear of the atoms can create twins, and lower the elastic energy in the system. As the strain rate increases, the size of the twins decreases and the number of twins increases. Beyond the critical strain rate, amorphization occurs, and the specimen deforms uniformly.

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