Key Engineering Materials Vols. 274-276 (2004) pp 331-336
Online available since 2004/Oct/15 at www.scientific.net

doi:10.4028/www.scientific.net/KEM.274-276.331

The Deformation of Nano-whiskers of Mono-crystalline Copper: Shape Effect, Properties, Shear Banding and Necking

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Keywords: Mechanical behaviour, shape effect, shear banding, copper nano-whisker, molecular dynamics

Abstract. This paper discusses some theoretical aspects in deforming nano-whiskers of mono-crystalline copper by uniaxial tension. With the aid of the molecular dynamics analysis, the present study revealed that the behaviour of a nano-whisker is very sensitive to its size, crystal orientation and geometry. The most stable surface is with (111) atomic structure and the most reliable whisker for testing is a hexagonal specimen composed of four (111) and two (100) surfaces and two $(1\bar{1}0)$ ends. The elastic modulus of a nano-whisker is very close to that of a micro-whisker but the ultimate tensile strength of the former is much higher. The mechanisms of shear banding and necking are far more complex than ever thought.

Introduction

A complete figure of the stress-strain behaviour of a nano-scale specimen under tensile loading is of primary importance to the development of nanotechnology. However, the information about the mechanical properties of nanoscopic specimens is lacking and the potential problems of testing such tiny specimens have not been explored, although there have been some investigations on the deformation of microscopic specimens. This is because adequate testing techniques are unavailable. On the nanometre scale, specimen preparation becomes very difficult and a mechanical testing must be well controlled with a high level of stability in terms of temperature, strain rate, crystal orientation and shape of specimen. On the other hand, a material can no longer be treated as a continuous body theoretically so that the powerful theory of continuum mechanics does not apply.

The molecular dynamics method has shown its unique advantage in analysing a variety of deformation problems on the nanometre scale. It has been applied successfully in characterising the deformation of metals [1-5], semi-conductors [6-9], chemical effect [10], carbon nanotubes [11], thin films [12] and liquids [13] and therefore will be used in this study to investigate the deformation of copper nano-whiskers subjected to uniaxial tension. Some important aspects, such as those of shape and atomic orientation, will be discussed in detail to provide the theoretical basis for potential experimental testing.

Molecular Dynamics Modelling

A molecular dynamics model based on the Morse potential is reliable for investigating the deformation of copper [2-5] and will be used in this study. In the Morse potential,

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$$\phi(r_{ij}) = D\left[e^{-2\alpha(r_{ij} - r_0)} - 2e^{\alpha(r_{ij} - r_0)} \right], \tag{1}$$

r_{ij} is the interatomic separation between atoms i and j, r_0 is the equilibrium separation at which the potential minimises. D and α are material constants listed in Table 1. The physical meaning of D is the cohesive energy between the two atoms.

Table 1 Parameters in the standard Morse potential.

Parameter	Cu-Cu
D (eV)	0.342
α (nm^{-1})	13.59
r_0	0.287

With the above potential, the forces on atom i due to the interaction of all the other atoms can be calculated by

$$F_i = -\sum_{j=1,\, j\neq i}^{N} \Delta_i \phi(r_{ij}) \tag{2}$$

where N is the total number of atoms in the model, including thermostat and boundary atoms. Consequently, the motion of all the Newtonian atoms in the control volume, including their instant position and velocity vectors, can be obtained by following the standard procedures of molecular dynamics analysis [14].

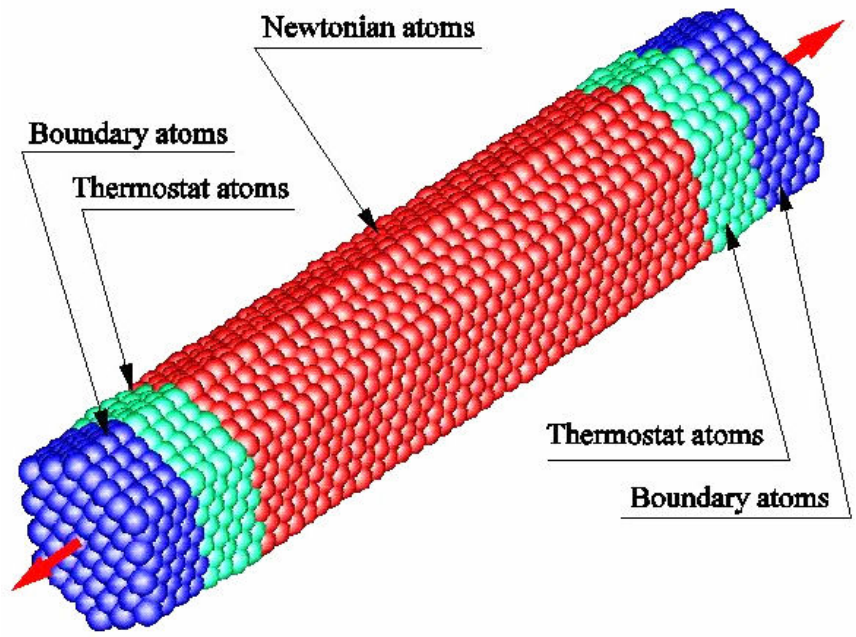


Fig.1 The molecular dynamics atomic model of a hexagonal nano-whisker specimen of mono-crystalline copper

For increasing the computational efficiency, a basket of neighbouring atoms with 14 units was maintained for each atom while the Morse potential cut-off radius was taken as 9 units. The basket was updated adequately within certain time interval by considering both the accuracy and efficiency. A criterion used for updating was that an atom which was not in the basket does not enter the Morse potential cut-off radius or an atom which was within the cut-off radius does not leave the basket before a further updating. The motion of an atom depends on the strain rate of testing and thus a higher strain rate needs a larger basket.

Figure 1 shows the initial atomic configuration of a specimen with a hexagonal cross-section. To maintain properly the temperature at 298°K during MOLECULAR DYNAMICS simulation, thermostat atoms were arranged at the two loading ends of the specimen, which absorb the rise in velocity momentum of Newtonian atoms. The scaling of velocities of the thermostat atoms was done by

$$V_{new} = V_{old}\sqrt{\frac{\text{Kinetic energy corresponding to the environmental temperature}}{\text{Kinetic energy of a thermostst atom before scalng}}} \tag{3}$$

where V_{new} is the scaled velocity of a thermostat atom and V_{old} is its original velocity.

Results and Discussion

Effect of Atomic Orientation and Specimen Shape. When a simple square model with (100) lattice in the direction of loading is subjected to free relaxation, a shrinkage of about 23% occurs. The surface atoms tend to restructure to (111) to maximise its atomic density, while those in the core of the specimen remain in a stable FCC configuration of (100). As a result, a shrinkage stress is generated before the uniaxial tensile loading. Table 1 shows that the shrinkage stress is sensitive to the dimensions of nano-whiskers and smaller specimens have higher shrinkage stresses. This is because on the nanometre scale a specimen always tends to deform in a manner that may minimise its net potential energy.

In an FCC structure, atomic lattices in different directions have different atomic densities. It is therefore not difficult to understand that specimens with different shapes and surface orientations would have different dimensional stability and shrinkage stress. The above observation suggests that the shape of a specimen may be stabilised so that the shrinkage stress can be minimised by maximising the surface atomic density. A systematic investigation shows that a specimen with a uniform square cross-section of two (111) and two $(11\bar{2})$ surfaces has a less shrinkage stress. A specimen, oblique in shape, with all its four surfaces as (111) planes shows an even less distortion during relaxation. The best specimen shape is with a hexagonal section, which has four (111) and two (100) surfaces, as shown in Fig. 1. Such specimens do not have sharp edges, can maximise the gross density of the atoms on the surfaces and minimise the distortion and shrinkage stress. Thus this type of specimens is highly recommended for actual testing.

Elastic Modulus and Ultimate Tensile Strength. With most materials, there is a gradual transition from elastic to plastic deformation and the onset point of plastic deformation is difficult to define with precision on the macroscopic or microscopic scale. For a nano-specimen, however, plastic deformation can be said to have occurred when an atom has changed its position permanently, *e.g.*, when a single dislocation takes place. The last column of Table 2 indicates the strain needed for the occurrence of the first predominant slip in different specimens and directly gives rise to the modulus of elasticity. The modulus of elasticity, using the most stable hexagonal specimen, is found to be 120 GPa, which is very close to that of 130 GPa obtained by a macroscopic engineering test. This indicates that macroscopic

testing can be used instead of the difficult nanometre-scale experiment, if the measurement of elastic modulus is the only concern.

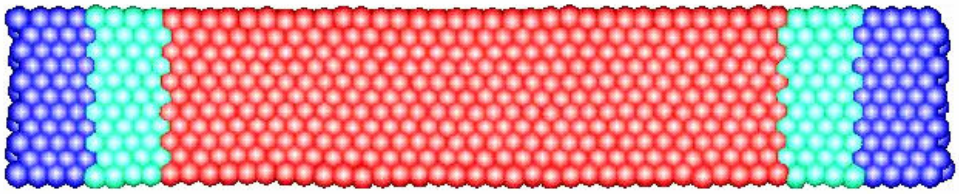
It is the fact that the ultimate tensile strength (UTS) in a single crystal can be some times higher than that of the same poly-crystalline material, tested at the same temperature and strain rate. A distinct rise in UTS has also been observed when the size of specimens reduces to the microscopic scale, for instance, to a micro-whisker as small as 6.8μm in diameter, which shows a UTS of about 1950 MPa as against that of 220 MPa measured with macroscopic specimens of poly-crystalline copper. The present MOLECULAR DYNAMICS simulation further shows that the UTS of a nano-whisker of a single crystal copper can go up to 6000 MPa, which is about three times the strength of a micro-whisker.

Table 2 Effects of size, shape and surface atomic structure of copper mono-crystalline nano-whisker.

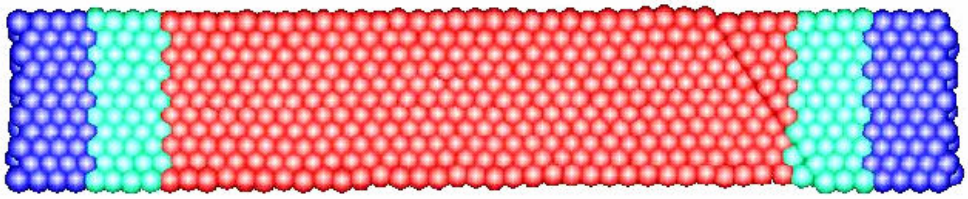
Specimen Cross-Sectional Shape	Specimen Size (unit cell)	Atom Number in Specimen	Shrinkage Stresses Generated (MPa)	Ultimate Tensile Strength (MPa)	Strain at the Onset of Plastic Deformation
Specimen with a rectangular cross-section and (100) surfaces	10×1×1	263	9000	14000	12.5
	30×2×2	763	7500	9000	6.9
	30×2×4	1373	4000	8100	8.0
	30×4×4	2471	3000	9100	18.2
	30×4×8	4667	1500	8200	15.8
	30×8×8	9971	750	6400	7.4
	34×8×16	19355	500	-	-
Specimen with a hexagonal cross-section	48×9×7	3871	0	6000	5.5

Mechanism of Shear Banding and Necking. Although the theory of shear band formation has been well established, little knowledge is available to fully explain the actual mechanism as to how a band begins to form.

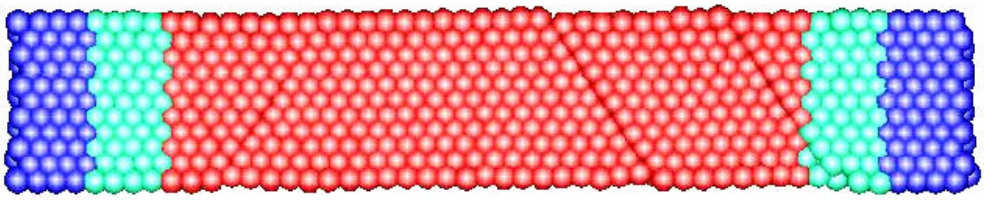
Figure 2 shows the evolution process of shear banding and necking revealed by the present molecular dynamics simulation. Even in the elastic stage, the deformation in the atomic lattice has been non-uniform, see Fig.2 (a). Figures 2(b) to 2(c) show that the first and second shear bands occur when the built-up stress is gradually released. The process of stress build-up and stress release continues in the whole elastic-plastic deformation process when the total strain varies from 5.64% to 11.33%. By this time all the primary shear banding forms. A further straining, as shown in Fig. 2(d), brings about the onset of necking at one of the weaker zones between two bands. In conjunction with this, stress increases first and then drops quickly when a noticeable necking forms. One may conclude at this stage that the necking would proceed further. It is unfortunately not true. The atoms in the zone of the above first necking are quickly restructured by minimising their potential energy and exhibit a stronger resistance to further deformation. As a result, a second necking takes place between other bands, as shown in Fig. 2(e). This process continues until a prominent slip occurs, as shown in Fig. 2(f), which leads to a stable necking followed by the final breakage of the specimen.



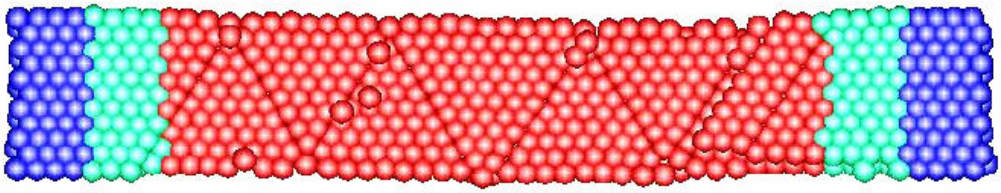
(a) At the strain of 4.61%.



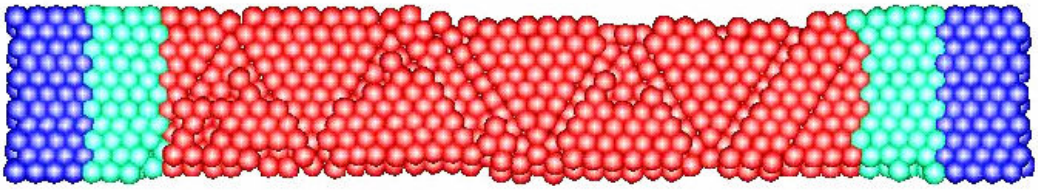
(b) At the strain of 5.64%. Note the formation of the first shear band near the right end.



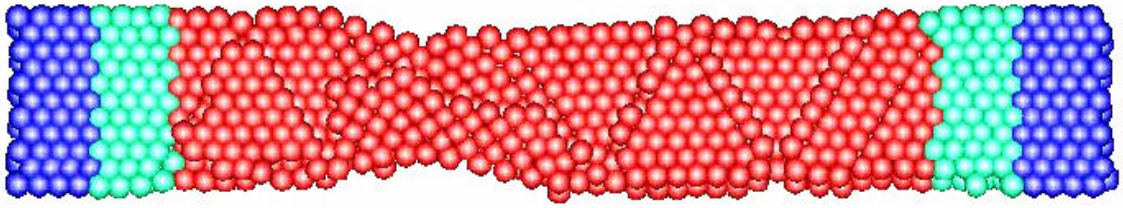
(c) At the strain of 6.36%. Note that the second shear band has formed.



(d) At the strain of 11.4%. Note that many shear bands have formed. Non-uniform cross-section shrinkage can now be observed clearly at this stage.



(e) At the strain of 14.15%. Note that at this stage, non-uniform cross-sectional shrinkage has appeared in a number of places in the specimen. Necking appears at several locations along the specimen.



(f) At the strain of 15.59%. Note that the location of necking is stabilised.

Fig.2 The evolution process of shear banding and necking in a nano-whisker of mono-crystalline copper under uniaxial tension. The results are from molecular dynamics simulation of the hexagonal specimen specified in Table 2. These are the cross-sectional views through the centre of the whisker specimen.

Conclusions

The above investigation leads to the following new understandings:

1. A hexagonal nano-whisker with four (111) and two (100) side surfaces should be used for testing to achieve a high level of shape stability and eliminate the effect of shrinkage stress.
2. Elastic modulus on the nanometre scale is close to that from macroscopic measurement.
3. The ultimate tensile strength increases as the size of a specimen decreases. We have demonstrated that an ultimate tensile strength of 6 GPa can be reached.
4. The mechanisms of shear banding and necking on the nanometre scale are much more complex than previously thought. Shear bands form with sequence and the stabilization of necking location depends on shear band development.

Acknowledgments

The authors would like to thank the continuous support from the Australian Research Council to this research through its ARC Large Grant Scheme.

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Advances in Engineering Plasticity and Its Applications
doi:10.4028/www.scientific.net/KEM.274-276

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