A multiscale deformation analysis for mono-crystalline copper under dynamic uniaxial tension

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Abstract. This paper presents a concurrent multiscale study for the deformation mechanism of mono-crystalline copper under dynamic uniaxial tension. The multiscale simulation is based on the coupled meshless and molecular dynamic (MD) method. Using it, the size of computational model can be extended to a large dimension (in micrometer) with an atomistic resolution. The pure MD simulation is difficult to reach this microscopic dimension because the number of atoms will be too large. In this study, it has been revealed that the deformation behavior and mechanism of the copper is sensitive to its size, geometry, and loading strain rate. In addition, the Young's modulus is found to be independent of the cross-sectional size and the strain rate range considered in this study. On the other hand, the yield stress decreases with specimen length and increases with the loading strain rate.

Keywords: copper; deformation mechanism; multiscale; molecular dynamics; meshless method.

Introduction

In the advanced nanotechnology and science, multiscale modeling and simulation are becoming more and more important, because in many cases, it is essential to understand the deformation mechanism across several length scales from nanoscopic to macroscopic. The individual modelling techniques are inapplicable to handle these problems. Therefore, the computational multiscale techniques have been proposed [1,2,3]. Gu and Zhang [1] developed a multiscale technique based on the combination of the Molecular Dynamics (MD) and the meshless method. We will use this coupled MD/Meshless technique in this paper.

This paper presents a concurrent multiscale study for the deformation mechanism of mono-crystalline copper under dynamic uniaxial tension. An advanced transition algorithm using transition particles was employed to ensure the compatibility of both displacements and their gradients [1]. Using this multiscale modeling technique, the size of computational model can be extended to the microscopic dimension (in micrometer) with an atomistic resolution. The pure MD simulation is difficult to reach this microscopic dimension because the number of atoms is too large [2,3].

Multiscale computational modeling

In the multiscale analysis as shown in Fig. 1, a problem domain is divided into a continuum domain Ω^c and an atomic domain Ω^a. These two domains are joined by a transition region Ω^t. The meshless method is used for the continuum domain, and MD is used for the atomic domain. The smooth combination of mechanics quantities in these two domains is achieved by the introduction of transition particles, which are totally independent of the meshless field nodes and the MD atoms.

In the transition region Ω^t, there are displacement compatibility and force equilibrium in coupling Ω^c and Ω^a:

$$\mathbf{u}_k^c = \mathbf{u}_k^a, \quad \mathbf{f}_k^c + \mathbf{f}_k^a = 0 \tag{1}$$

where $\mathbf{u}_k^c$, $\mathbf{f}_k^c$ $\mathbf{u}_k^a$, and $\mathbf{f}_k^a$ are displacements and forces at a transition particle *k* obtained by the continuum method and the atomic method, respectively. It will be ideal to satisfy both the displacement compatibility and the force equilibrium conditions, but the displacement compatibility is the most important and must be satisfied.

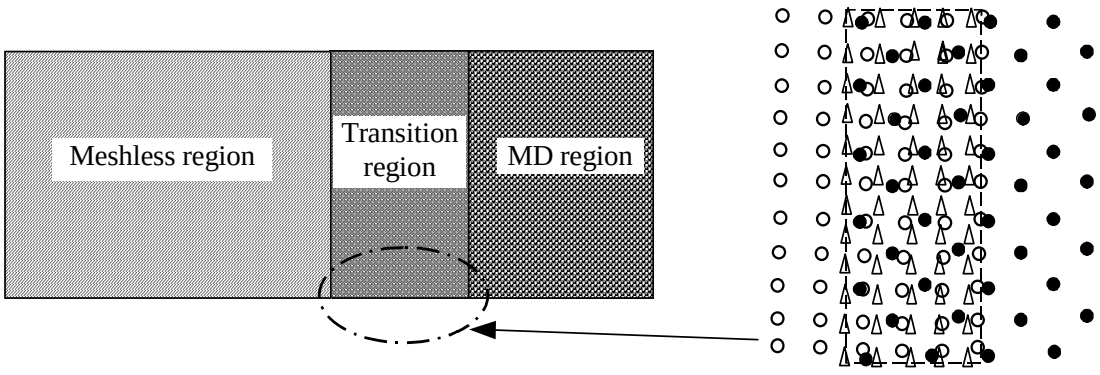

Figure 1 The computational multiscale modeling

To satisfy the displacement compatibility condition, several handshaking strategies have been developed. Following the idea of the bridging domain method [4], a newly developed transition technique [1] is used to ensure a seamless transition between the continuum domain and the atomic domain. As shown in Fig. 1, several layers of transition particles are inserted into the transition region to ensure the compatibility conditions and facilitate the energy

exchange from Ω^a to Ω^c. The displacement compatibility condition between atoms and meshless nodes is achieved through these transition particles. The kinetic energy and potential energy of continuum domain will first be transmitted to these transition particles and then to the atomic domain, and *vice versa*. This transition algorithm allows the continuum nodes to become independent of the atoms. In addition, the compatibility conditions in the transition domain can be conveniently controlled through the adjustment of the number and distribution of the transition particles.

Since the frequency of the atomic domain is much higher than that of the continuum domain, the multiple-time-step algorithm is more favorable, both computationally and physically. Hence, we will use this algorithm, in which a larger time step is used in the continuum domain but a finer time step is used in the atomic domain. Let ΔT^c be the time step for the continuum domain and Δt^a be the time step for the atomic domain. We use $\Delta T^c = N\Delta t^a$.

Multiscale study for mono-crystalline copper under dynamic uniaxial tension

Figure 2 shows a computational model for a mono-crystalline copper bar under dynamic uniaxial tension. The model size is around 3×116 nm, and it has a large dimension in x direction. If the pure MD is used, about 11000 atoms are required. In the multiscale simulation, the central part is simulated by MD and the other parts are handled by the meshless method. Hence, only 296 continuum nodes and 1920 atoms are used. In addition, 600 transition particles are required in the transition region. The save for the computational cost is significant.

The dynamic (with different strain rates) displacement boundary conditions are applied to the two ends of the copper bar. The up and bottom surfaces are free. The deflection of the copper bar increases with loading strain. When the deformation is large enough, necking and dislocation can be clearly seen from Fig. 3.

To study the strength of this mono-crystalline copper bar, the stress-strain curve is obtained and plotted in Fig. 4. From this curve, it can be seen that the mono-crystalline copper have good elongation property[5]. The strain can reach about 15% of the original length. At the beginning stage of stress-strain curve, the deformation is elastic and the specimen will return to its original shape when the applied stress (strain) is removed. When the stress continually increases to a certain value (the yield stress), the material begins to deform plastically. When stress is larger than the ultimate stress (or ultimate strength) (US), the material will be failure.

Form Fig. 4, we can see that the ultimate strength of this mono-crystalline copper bar is around 11Gpa, which is much higher than that in macro-scale. It is because mono-crystalline copper has no defects. We can also obtain from this figure that Young's modulus is around 90GPa which also much larger than that obtained in macro-scale.

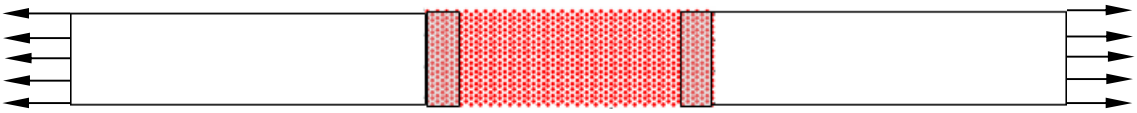

Figure 2 Mono-crystalline copper under uniaxial tension

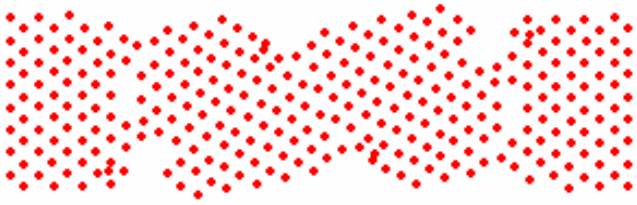

Figure 3 The deformation (when close to failure)

The influences of model sizes and loading strain rates are also studied. It can be found that a larger cross-section supports higher stress level, but a longer model has a smaller ultimate stress. However, Young's modulus is almost that same for different model sizes.

Fig. 5 plots the stress-strain curves for different loading strain rates. It can be found that a higher strain rate supports higher stress level, therefore, higher ultimate stress. Again, Young's modulus is almost independent of the loading strain rates.

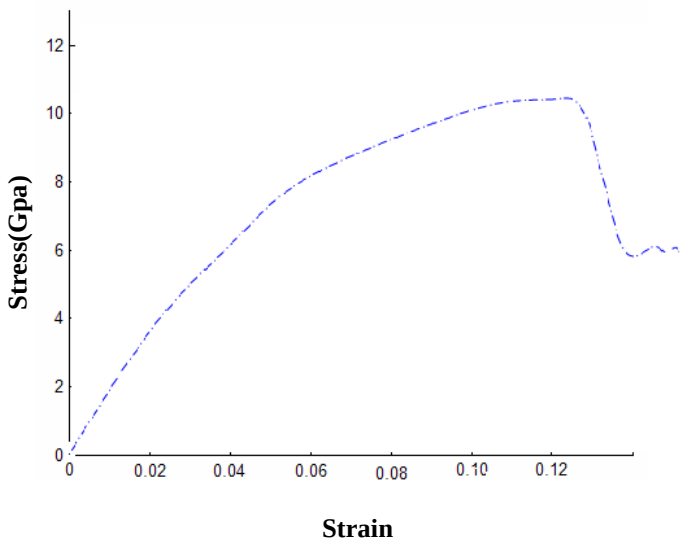

Figure 4 The stress-strain curve

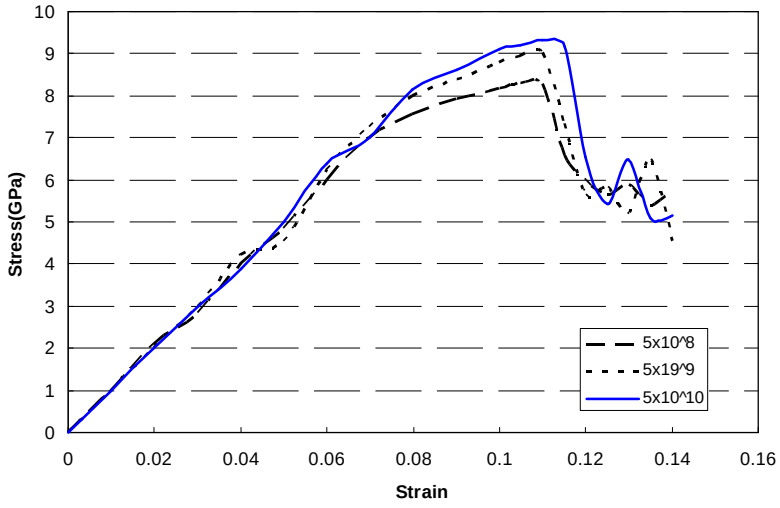

Figure 5 The stress-strain curves for different loading strain rates

Conclusion

The deformation mechanism of mono-crystalline copper under dynamic uniaxial tension is studied using the concurrent multiscale technique. In this multiscale simulation, the size of computational model can be extended to the microscopic dimension (in micrometer) with an atomistic resolution. It has found that the mono-crystalline copper has very good elongation property and the ultimate strength is much higher than that obtained in macro-scale. It has

been revealed the ultimate stress and the yield stress decrease with the specimen length and increase with the loading rate. However, Young's modulus is found to be independent of the cross-sectional size and the strain rate range considered in this study.

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