Effect of void orientation on void coalescence during dynamic fracture of metals: a molecular dynamics study

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ABSTRACT

The effect of void orientation on void coalescence in a three-dimensional single-crystal face-centered-cubic lattice has been studied. Molecular dynamics simulations using an embedded-atom potential for copper have been performed at room temperature and using uniaxial tensile strain controlling with strain rates $10^{10}$/sec. Void growth has been simulated in three different orientations, namely, 0 degree, 45 degrees, and 90 degrees void configuration. The correlated growth of the voids during their linking is investigated both in terms of the onset of coalescence and the ensuing dynamic interactions the reduction of the distance between the voids and the directional growth of the voids. Von Mises stress and total potential energy are plotted, which change rapidly around the onset of the void coalescence.

Key words: Copper, Dynamic fracture, Void coalescence, Molecular dynamics, Strain rate, MD++, Periodic boundary condition

1. INTRODUCTION

Ductile fracture of metals commonly occurs through the void nucleation, growth, and coalescence of microscopic voids as seen in Fig.1. Initially voids nucleate from the weak points in the material such as inclusions and/or grain boundary junction. Once voids are nucleated, the voids grow under the tensile stress, driven by the reduction in elastic energy. Eventually, the voids grow sufficiently large that they interact with each other, coalesce into larger voids, and finally form the fracture surface [1, 2].

Computationally void growth has been studied extensively at the continuum level, and more recently at the atomistic level. The atomistic studies demonstrate that voids grow by
emitting dislocations, which carry away the material, platelets of atoms, from the void and are responsible for the plastic deformations needed to accommodate significant void growth.

There are also many recent studies of fracture in ductile metals with several holes or voids. While these studies model the void growth explicitly, often with fairly sophisticated models of plasticity, they typically simplify the coalescence process to instantaneous unification of the voids based on a relatively simple criterion such as growth of the voids to within one void diameter of each other or a plastic strain threshold. The earlier continuum studies and the one atomistic study known to us of the coalescence process have been conducted in effectively two-dimensional and highly symmetric systems [5].

A particularly interesting case is the dynamic fracture of ductile metals, in which the strain rates are so high that processes such as diffusion operating on relatively long-time scales may be neglected, while inertial effects become relatively important [3].

In this study of dynamic fracture in ductile metals at a high strain rate $[10^{10}\text{/sec}]$, we have performed molecular dynamics (MD) simulations in single crystal face-centered cubic (FCC) systems using EAM (Embedded-Atom Model) potential for copper.
2. METHOD AND SIMULATIONS

In this atomistic-level study of void growth, the molecular dynamics simulations have been done using MD++. The system, in which the simulations are done, is a three-dimensional single-crystal face-centered-cubic (fcc) in a cubic box with \{100\} faces.

The volume of the cubic box is 1000\text{nm}^3 and the box contains 87440 atoms and each except two voids. Periodic boundary conditions are used in all the three directions so that there are no free boundaries in the system apart from the voids. Equivalently the system can be imagined to consist of an infinite periodic array of voids. Three systems that have two identical spherical voids oriented 0, 45, and 90 degrees respectively in the center were modeled.

Fig.2. the snapshots of the sliced view of the systems

10^{10}/\text{sec} true strain rate was applied along y-axis (vertical direction) while control the temperate at T = 300 K with Nose-Hoover thermostat. One step of simulation that gives 1% strain in a picosecond took about 40 minutes by our computer resources, one desktop (Pentium 4 CPU 3.2 GHz 2GB RAM ) and two laptops (Pentium M CPU 1.6 GHz 512MB RAM). 15 steps for each systems were simulated. Atomeye was used for the post-process.
3. RESULTS

Figure 3 shows the sequence of void coalescence for 0 degree voids system from 8% to 13% strain. Voids didn’t change much below 8% strain. Voids coalesce at 10% strain and void size increases rapidly as the dislocations generate and propagate beside each void horizontally. We can see dislocations propagate 45 degrees, which is the direction where maximum stress occurs.

The corresponding images of Von Mises shear strain are in Fig 4. Bright colors on the voids surface indicate higher shear strain, and the blue is for the lower strain. Shear strain concentrates in the center of two voids from 8% to 10% while plastically deformed area get lager around the voids. After voids coalesce at 10% strain, concentrated shear strain is diffused out.
Fig. 4. Visualization of Von Mises shear strain for 0 degree voids system

Fig. 5. The sequence of void coalescence for 45 degree voids system
Fig. 5 and 6 are for the 45 degree voids system. Voids coalesce at 10% strain. It is the same value as that of the 0 degree, but after the void coalescence, the 45 degree system fails more catastrophically than 0 degree system. Two main diagonal dislocations are apparent in the snapshot of Von Mises shear strain at 11% strain.

Fig. 7 and 8 show the process of void coalescence for 90 degree voids system. Voids coalesce at 12% strain, two steps later than those of 0 and 45 degrees. 90 degree voids system is most stable against the fracture among three.
Fig. 7. The sequence of void coalescence for 90 degree voids system

Fig. 8. Visualization of Von Mises shear strain for 90 degree voids system
Finally, void coalescence initiates at 10% strain for both 0 degree and 45 degree systems, and 12% for 90 degree system. Failure of the ductile metal accelerates rapidly after the void coalescence. Yield in ductile materials is usually caused by the slippage of crystal planes along the maximum shear stress surface. Therefore, a given point in the body is considered safe as long as the maximum shear stress at that point is under the yield shear stress \( \sigma_y \) obtained from a uniaxial tensile test.

The von Mises Criterion often used to estimate the yield of ductile materials. The von Mises criterion states that failure occurs when the energy of distortion reaches the same energy for yield/failure in uniaxial tension. Mathematically, this is expressed as,

\[
\bar{\sigma} = \left[ \frac{1}{2} \left( (\sigma_{11} - \sigma_{22})^2 + (\sigma_{11} - \sigma_{33})^2 + (\sigma_{22} - \sigma_{33})^2 + 3\left(\sigma_{12}^2 + \sigma_{13}^2 + \sigma_{23}^2\right)\right) \right]^{\frac{1}{2}}
\]

Instead of the stress-strain curve, Von Mises stress-strain curve is plotted in Fig. 9 to show the correlation between void coalescence and mechanical failure of the ductile material. The stresses needed to get the Von Mises stress was collected from stress tensor by each calculation result of MD++. Von Mises stress increases linearly until the voids coalesce. After the void coalescence Von Mises stress decreases rapidly.

\[
\text{Stress tensor: } \sigma_{ij} = \begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{bmatrix}
\]

Rapid changes in the total potential energy also correspond to the void coalescence at 10% for 0 and 45 degrees, and 12% for 90 degree.
Fig. 9. the potting for true strain vs. Von Mises stress

Fig. 10. the plotting for true strain vs. total potential energy
REFERENCES