

Molecular Dynamics Study of Void Growth and Dislocations in dynamic Fracture of FCC and BCC Metals

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MOLECULAR DYNAMICS STUDY OF VOID GROWTH AND DISLOCATIONS IN DYNAMIC FRACTURE OF FCC AND BCC METALS

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ABSTRACT Void growth with concomitant dislocation formation has been studied in single crystal face-centered-cubic and body-centered-cubic metals using molecular dynamics method with Embedded-Atom and Finnis-Sinclair potentials for copper and tantalum, respectively. We have concentrated on the quantitative analysis of the void shape evolution, on the structure of dislocations, which emerge from the void, and on the continuum measures such as plastic strain. The effects of strain-rate, differences between lattice structures, and loading conditions as uniaxial, biaxial, and triaxial expansion on the shape of the void and on the dislocations have been investigated.

INTRODUCTION: In ductile fracture of metals rupture can be induced by spallation, in which two reflected shock waves, created when a flyer hit a target material, cross and create a large tension leading to the fracture in the target sample [c.f. Kanel et al. 1986]. The fracture typically begins by nucleation, growth, and coalescence of voids. In this study we concentrate on void growth in dynamic fracture of metals with concomitant dislocation formation. The strain-rates ($\dot{\epsilon}$) used here are high, ranging from 10^7 /sec to 10^{10} /sec. The lowest of these strain-rates can be studied with spallation experiments, e.g. using shock-loading with lasers.

METHOD: The investigation has been carried out using molecular dynamics (MD) which enables us to study the evolution of the void and the dislocations emerging from the void at the atomistic level. The simulations have been mainly done using empirical Embedded-Atom (EAM) potentials [Oh *et al.* 1989] to model copper and have been performed using a cubic simulation box with periodic boundary conditions. The box is oriented along the $\langle 100 \rangle$ directions of a single crystal face-centered cubic (FCC) lattice created by replicating 60 FCC unit cells along each of the cubic axes giving total 864000 atoms. The system has been evolved with a thermostat on to bring it to equilibrium at room temperature ($T=300\text{K}$) and ambient pressure. At equilibrium the box has a side length of 21.7nm. After the system is brought to equilibrium a spherical void is cut at the center of the simulation box. The radius of the void has been varied between 1nm and 3nm. Then the thermostat is turned off and the expansion is applied by rescaling the distances between the atoms in each time step [Belak 1998]. Three different loading modes have been applied, namely uniaxial, biaxial, and triaxial. Also body-centered-cubic (BCC) metals such as tantalum

have been studied using Finnis-Sinclair potentials [Finnis *et al.* 1984] for systems of comparable size with the case of copper.

The stress-tensor is computed microscopically using the virial formula:

$$\sigma_{\alpha\beta} = \frac{1}{V} \left(\sum_i p_{i\alpha} p_{i\beta} / m_i + \sum_i \sum_{j>i} r_{ij\alpha} F_{ij\beta} \right), \quad (1)$$

where p_i is the component of the momentum of an atom i with the mass m_i , and r and F are the interatomic distance and force of a pair (ij) . Also, the location and character of defects including the void surface and dislocations are computed using techniques developed for finite temperature. The shape evolution of the void is characterized using multipole moments from spherical harmonics.

RESULTS AND DISCUSSION: From the stress-tensor the mean stress, $\sigma_m = 1/3 \text{ Tr } \sigma$, and Mises stress, $\sigma_e = [3J_2]^{1/2}$, where J_2 is the second variant of the stress deviator $\sigma = \sigma_{\alpha\beta} - \sigma_m \mathbb{I} \delta_{\alpha\beta}$, are derived. The effect of the stress-triaxiality,

$$\chi = \sigma_m / \sigma_e, \quad (2)$$

is of particular interest. From the simulations also continuum measures as plastic strain can be calculated, $\dot{\epsilon}_{\alpha\beta}^P dt = \dot{\epsilon}_{\alpha\beta} dt - \dot{\epsilon}_{\alpha\beta}^E dt$, where the elastic strain increment is derived using the elastic compliance tensor, $\dot{\epsilon}_{\alpha\beta}^E(\sigma_{\alpha\beta}) = S(\sigma_{\alpha\beta}) \dot{\sigma}_{\alpha\beta}$. Having the stress and plastic strain tensors the plastic work is also measurable. From the microscopic void analysis the porosity, f , *i.e.*, the ratio of the void volume to the total volume, is calculated, too.

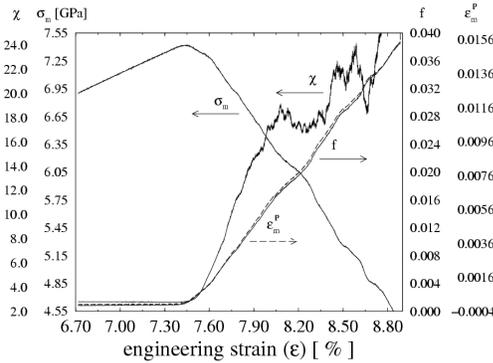


Figure 1: Mean stress (σ_m), stress-triaxiality (χ), porosity (f), and mean plastic strain (ϵ_m^P) versus engineering strain (ϵ) in a single crystal copper with a pre-existing void under uniaxial dilational strain at strain-rate 10^8 /sec.

Some of the quantities defined above and measured from the calculations are plotted in Fig. 1 for a single crystal copper, whose radius of the void is 1nm, and have been

under uniaxial dilational strain. As can be seen from the figure the porosity and mean plastic strain follow each other precisely. This equivalence is comparable with continuum calculations, where the matrix materials are assumed to be elastically rigid and plastically incompressible [Gurson 1977]. The behavior of the system under loading can be divided in three regimes: first the system expands elastically, stress increases nearly linearly, and stress-triaxiality and porosity stay constant. At yielding the mean stress drops and the stress-triaxiality grows rapidly from the value of $\chi = 3.0$, which can be derived also from the elastic constants for copper, to a value of $\chi = 22.0$, thus the stress-state in the system becomes more triaxial. At the same time the porosity and mean plastic strain increase linearly. After stress-triaxiality has reached a value of about 22.0, it saturates until failure.

The quantitative analysis of the void shape evolution shows that the void, when under uniaxial loading is first slightly elastically expanded in the direction of the load. When yielding starts it makes a rapid shape-change and expands more to the opposite directions than the load. Finally the void develops an octahedral shape. In the simulations with biaxial and triaxial loading, the octahedral shape is more profound and the void shape more isotropic. Dislocation activity in the system differs greatly depending on the loading mode: in the uniaxial case there are fewer active glide planes and stacking fault ribbons are broader than in the biaxial or triaxial cases. When comparing the BCC and FCC lattices, the temperature should be higher and/or strain-rates lower in BCC in order to see nice dislocation formation. The parallelogram shapes of the prismatic loops formed by the dislocations in FCC lattices differ from the more triangular shape in the case of BCC tantalum.

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