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FINITE-TEMPERATURE NANOVOID DEFORMATION IN COPPER UNDER TENSION

M.P. ARIZA*, M. PONGA*, I. ROMERO† AND M. ORTIZ‡

*Escuela Técnica Superior de Ingeniería
Universidad de Sevilla
Camino de los descubrimientos, s.n. 41092-Sevilla, Spain
e-mail: mpariza@us.es, mponga@us.es, http://grupo.us.es/gingest/

†Escuela Técnica Superior Ingenieros Industriales
Universidad Politécnica de Madrid
José Gutiérrez Abascal, 2, 28006 Madrid, Spain
e-mail: ignacio.romero@upm.es

‡Engineering and Applied Sciences Division
California Institute of Technology
1200 E. California Blvd. Pasadena, 91125 CA, USA
e-mail: ortiz@aero.caltech.edu, http://aero.caltech.edu/ ortiz/index.html

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Abstract. Tensile failure of metals often occurs through void nucleation, growth and coalescence. In high-purity metals, void nucleation often operates at the nanoscale and is followed by plastic cavitation when the void attains the critical size for dislocation emission. This work is concerned with the study of plastic nanovoid cavitation in face-centered cubic (fcc) crystals at finite temperature. In particular, the Quasicontinuum (QC) method, suitably extended to finite temperatures (HotQC), is taken as the basis for the analysis. The Quasicontinuum method is a multiscale modeling scheme that seamlessly links continuum and atomistic descriptions. HotQC is a method for systematically coarse-graining atomistic models at finite temperature. We specifically focus on nanovoids in copper single crystals deforming in uniaxial and triaxial tension. The results of the calculations provide a detailed characterization of the cavitation mechanism, including the geometry of the emitted dislocations, the dislocation reaction paths and attendant macroscopic quantities of interest such as the cavitation pressure as a function of triaxiality.

1 INTRODUCTION

In order to understand the mechanical response of materials subject to dynamical loads, the knowledge of the physical and thermodynamical properties of materials is required.Tensile failure of metals often occurs through void nucleation, growth and coalescence. This process, known as spallation, has been the subject of extensive metallurgical investigation [1]. In high purity metals, void nucleation often operates at the nanoscale and is followed by plastic cavitation when the void attains the pressure and temperature dependent critical size for dislocation emission. The voids grow through nucleation and motion of dislocations.

Molecular dynamics (MD) techniques have been used by many authors to understand the mechanical response of materials based on the mechanisms controlling the growth and evolution of nanovoids [2, 14]. However, a correct simulation of plastic phenomena requires the use of very large systems and appropriate boundary conditions, which may result in complex MD models. Computed plastic work during void growth indicate that there is a growth threshold controlled by the stress required to nucleate dislocation activity. The time-scale for complete dynamic fracture ($0.1-1\ \mu s$) is several orders of magnitude beyond the current limitations of molecular dynamics simulations. The study of slower strain rates, in the experimental range, requires much larger system sizes or a special continuum boundary condition. In this sense, multiscale modelling provides an alternative to MD simulation, especially for this type of problems.

The Quasicontinuum method (QC) is a multiscale modelling scheme that seamlessly links continuum and atomistic descriptions. In this paper we are going to use an extension of the static QC theory developed by [4] and subsequently adapted by [5], to systems in thermodynamic equilibrium and non-equilibrium (HotQC) established in [6]. Previous to this work, a number of finite-temperature extensions of QC were proposed within the framework of equilibrium statistical mechanics and thermodynamics [7, 8]. Whereas these formulations are effective for equilibrium problems, systems at uniform temperature, they cannot be applied to systems away from equilibrium. In [6] the probability density function of finding the system in a certain state is directly approximate by recourse to variational mean-filed theory and the *maximum-entropy* formalism. Every atom within the system has its own local statistical parameters, temperature and entropy. Therefore, the net result of the procedure is to define a *non-equilibrium free energy* depending on the positions and temperatures of all atoms. Conveniently, for several interatomic potentials of interest, including Lennard-Jones (LJ) and Embedded-Atom Method (EAM), the non-equilibrium free energy can be computed explicitly up to numerical quadratures, and the result may be regarded as a *temperature-dependent interatomic potential*. This structure greatly facilitates implementation, which is reduced to replacing ordinary interatomic potentials by temperature-dependent ones. It is worth emphasis that at no time in this procedure equilibrium statistical mechanics is invoked to define temperature and entropy or to determine the probability density function of the system. Thus, unlike the conven-

tional temperature and entropy defined in equilibrium thermodynamics and statistical mechanics, the local temperatures and entropies that arise in this theory are parameters that the mean-field probability density function is endowed with. For non-interacting atoms, the local temperatures and entropies do indeed coincide with the equilibrium values of each one of the atoms regarded as an isolated system in thermodynamic equilibrium, which justifies the use of terminology. Likewise, the non-equilibrium free energy is defined formally from the mean-field probability density function and reduces to the equilibrium free energy of the system when the temperature field is uniform.

Although experimental investigations [9, 10] indicate the existence of strong void size effects in plastic deformation of ductile materials with the growth of nanovoids, its experimental quantification remains an open problem. This size effect has been studied by [11] for periodic single crystals under different load conditions using discrete dislocation plasticity combined with a continuum strain gradient crystal plasticity theory. Similar techniques were applied by [12] to simulate the effect of lattice orientation on an isolated crystal with a cylindrical void.

Within the framework of MD, nanosized void growth in single crystal copper at finite temperature and high strain rates have been analyzed extensively. MD simulations of void growth at high strain-rate and room temperature [13], effect of stress triaxiality [14], void coalescence [15] have been carried out using the copper embedded atom method (EAM) potential due to [16]. More recently, [19] have studied the effect of loading orientation and initial void size at finite temperature using LAMMPS code and the EAM potential by [22].

Results are shown for numerical tests according to a non-equilibrium finite temperature problem using QC method. This problem has been studied by many authors, but none of them have included systems outside equilibrium. Also, the purpose of these tests is to understand the nucleation of particular arrangement of atoms around a nanovoid and the evolution of the temperature field in this process.

2 METHODOLOGY

2.1 The Quasicontinuum method (QC)

QC is a method for systematically coarse-graining lattice statics models. The method starts with a small and complete atomistic system around a core defect. Then the rest of the crystal is modelled in the geometry and reducing the configuration space of the crystal trough a judicious application of a finite element-based kinematic constraints. To avoid full lattice sums, only atoms in small clusters, surrounding the representative atoms must be visited for computing the effective out-of-balance forces. Additionally, the selection of representative atoms is performed adaptively based on the local strain of the elements. The tolerance governing the adaptation process is set so that the full atomistic resolution is attained only in the presence of dislocations.

The force among atoms is directly computed by empirical potentials. As in conventional

continuum mechanics, QC permits the direct simulation of systems controlled through the application of remote boundary conditions. Details of the implementation of QC used in the present study and an analysis of convergence of the method may be found in [4].

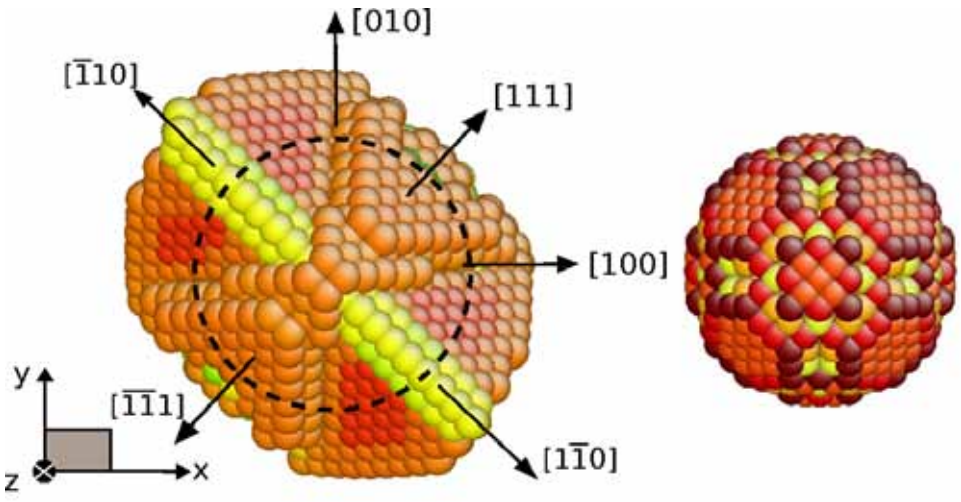

Figure 1: Initial void and incipient dislocation structures for the uniaxial loading simulation (load is applied in the [110] direction).

2.2 Equilibrium and Non-Equilibrium (HotQC)

The QC extension to systems in thermodynamic equilibrium and non-equilibrium (HotQC) was developed in [6] and extended to the study of nanovoids in single crystals for the first time in [20]. This extension is possible by the application of a variational mean-field theory and the maximum-entropy (*max-ent*) formalism. Using this formalism, we can directly approximate the probability density function to find the system in a certain state, not necessarily an equilibrium state. In this model, every representative atom has local state variables akin to temperature, entropy in addition to position, as parameters that determine the local statistics of the atom. Then, the *max-ent* variational principle provides the most likely probability density function within the assumed mean-field class and consistent with all constraints on the systems.

Attention to macroscopic processes that are quasi-static is performed. Under these conditions, the net result of the *max-ent* procedure is to define a non-equilibrium free energy depending on the positions and temperatures of all the atoms. The non-equilibrium free energy is computed explicitly by numerical quadratures and the result may be regarded as a temperature-dependent interatomic potential. The stable configuration of the system is found by minimization of the free energy for a given temperature field.

The next step in the development of the method therefore concerns the computations

of the evolving temperature field. We accomplish this by coupling the free-energy minimization problem to a diffusion form of the energy-balance equation. The proper form of the coupling is suggested by the variational formulation of coupled thermo-mechanics problems proposed in [21].

3 NUMERICAL TEST

We have carried out simulations under uniaxial and triaxial loading, using the empirical embedded-atom (EAM) potential due to Johnson [16]. For the uniaxial case, we consider a computational cell of size $432a_0 \times 432a_0 \times 432a_0$ ($a_o = 0.3615$nm) of copper, containing a total of 120×10^6 atoms. A spherical void of $7.5a_0$ radius is created in the center of the cell with initial full atomistic resolution within a $16a_0 \times 16a_0 \times 16a_0$ region surrounding the void. The initial mesh contains 4052 nodes after removing the atoms from the void. The external load consists of a uniaxial expansion in the [110] direction which provides the simplest dislocation configuration. We prescribe pure dilatational displacements on the external boundary (deformation is increased by steps of 0.2% increments) with the strain rate of $5 \times 10^7\ s^{-1}$. In every step of deformation a new stable equilibrium configuration is obtained by using the Polak-Ribière variant of the non-linear conjugate gradient algorithm. Previously to loading process the sample is allowed to expand isothermally at uniform temperature $T_0 = 300K$. In order to capture all the defects surrounding the void, we implement a routine that automatically remeshes the sample using the second invariant of the deviatoric part of the Lagrangian strain tensor as adaptivity indicator.

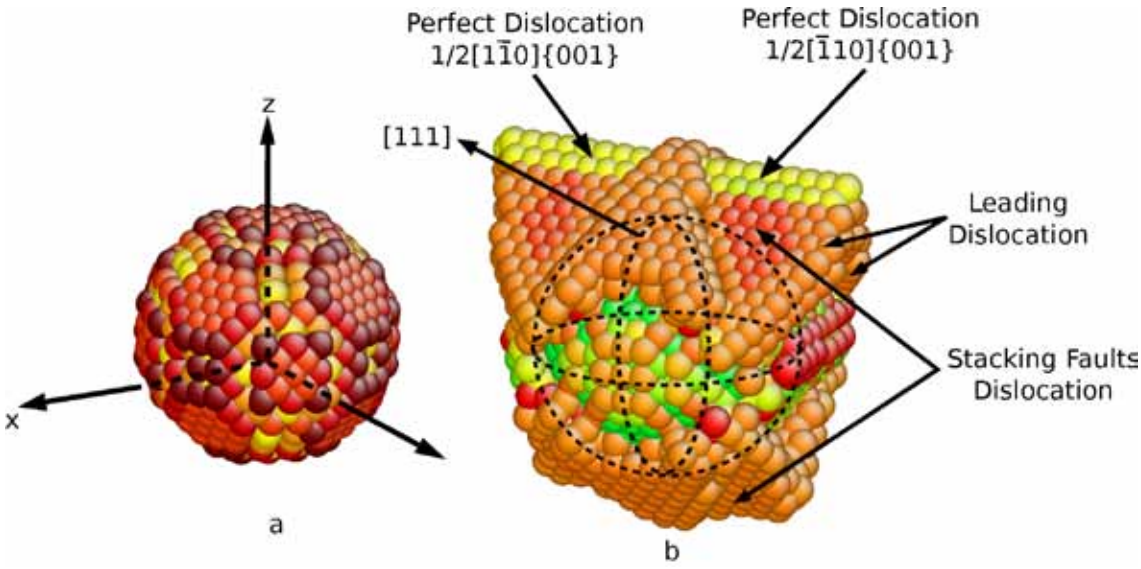

Figure 2: Isometric view of initial void and incipient dislocation structures. Stacking faults in {111} planes, perfect dislocations 1/2[110] in {001} planes and leading dislocations are observed.

During this uniaxial simulation, the void first becomes elongated in the direction of the

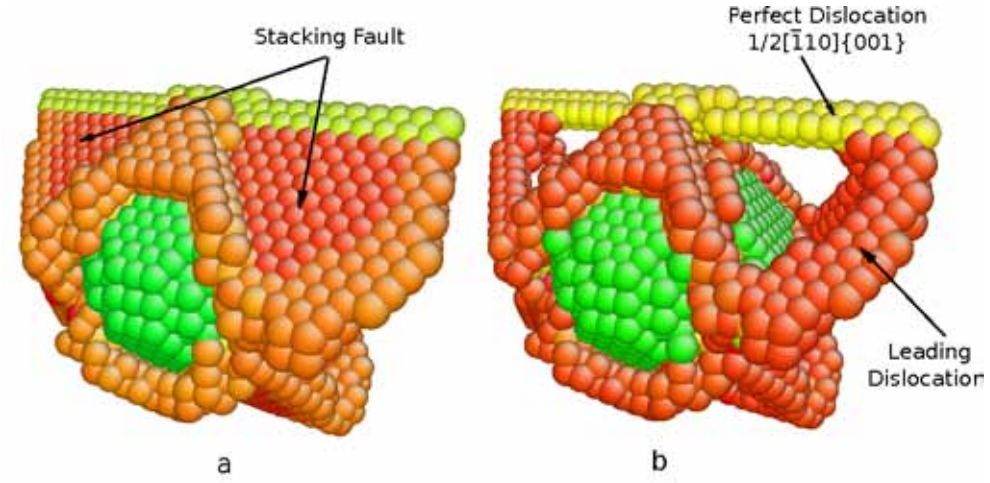

Figure 3: Initial stage of prismatic loop. This emission of dislocations is on the intersecting {111} planes have been predicted by [17]. a) Red atoms belong to stacking faults. b) Prismatic loop initiation (red) and perfect dislocation (yellow).

expansion without dislocation emission. In a second phase, dislocations grow around the surface of the void. The structures of the incipient dislocations are shown in Figs. 1 and 2. The vectors [111] and [$\bar{1}\bar{1}$1] indicate the plane of the stacking fault for FCC crystals. In Fig. 2 it is clearly seen the presence of stacking faults in {111} planes. On the intersection of these {111} planes, perfect dislocations labeled with 1/2[1$\bar{1}$0]{001} and 1/2[$\bar{1}$10]{001} appear. This first result agrees with the simulations presented in [17] and is the first step of the prismatic loop formation described in Fig. 1 in [18].

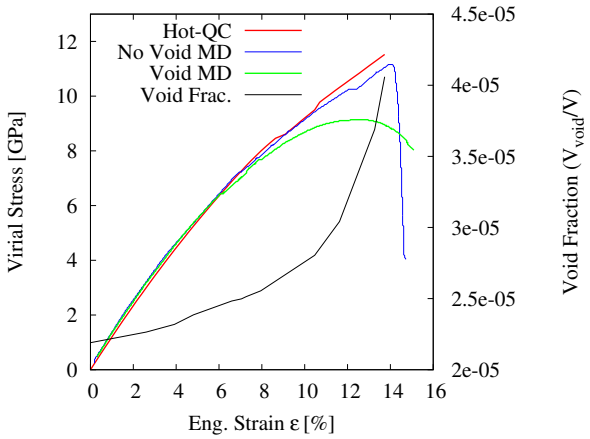

Figure 4: Computed virial stress for the uniaxial loading case compared with molecular dynamics simulations results [14] and normalized void volume expansion V_{void}/V vs deformation ε of the sample.

Once the prismatic loop is formed (Fig. 3), the loop emerges and moves away from

the void and is stopped when it reaches the limit of the atomistic region. This situation is obviously due to the computational mesh used in our simulations. Fig. 4 shows the stress-strain curve for the uniaxial loading simulation. We must note that the plotted strains and stresses are in the loading direction [110]. A comparison has been made with previous MD simulations of uniaxial loading in cooper [14] with loading direction [001] (see Fig. 4). It is noteworthy that the elastic moduli are in good agreement, and the linear regime is approximately up to 8% of deformation for both cases. In the plastic region, there is a difference probably due to the differences in the void size, the potential used and the loading direction, that activates different slip systems. The void fraction is also plotted in Fig. 4. At low deformations, the void grows approximately linearly up to 8% of deformation. Next, the void changes the rate of growth, and the behavior is approximately exponential as indicated by continuum theories.

In order to study the thermoplastic behavior of the material at high strain rates the triaxial loading case is simulated. The void dislocation emission analysis requires more attention, for this reason this study is out of the scope of this work. Additionally, the temperature of the atoms around the void when the fracture occurs is also studied.

Fig. 5 shows the stress-strain curves for the triaxial case. In this curve, a linear regime is observed up to 4% of deformation, followed by a non-linear regime representing the plastic work around the void. At this stage, the fracture mechanism is initiated and dislocations are emitted away from the void. When the deformation reaches the 6%, the void has a drastically change in shape and volume. This process is called *cavitation*. After this point, the stiffness of the sample decreases and the fracture extends all over the sample. The temperature evolution of this process is shown in Fig. 6. In this figure a first linear stage up to 4% of deformation is observed and is identified with the linear stage in the stress-strain curve. Then, up to 6% of deformation, a change in the slope occurs, corresponding to the non-linear stage. When the deformation reaches the cavitation point, and due to the breakage of atomic bounds the temperature increases. Atoms belonging to the void surface and near to the void show a higher increase rate of temperature. As the deformation increases, the temperature oscillates due to the successive breakage of bounds. The temperature of the atoms on the void surface to the void surface is approximately constant after cavitation. In contrast, the temperature of the atoms away from the void increases during the cavitation process.

4 CONCLUSIONS

In this work we have applied an extension of the QC method to study the thermomechanical behavior of a nanovoid under tension in copper. The extension of the Quasicontinuum method to non-equilibrium systems has provided a detailed solution of the forces, deformation, and temperature at every point of the sample, with atomistic resolution close to the defect. In this region, both adiabatic as well as isothermal simulations indicate that a fragile fracture occurs in the material shortly after dislocation structures appear. The multiscale resolution of the Quasicontinuum approach then serves to com-

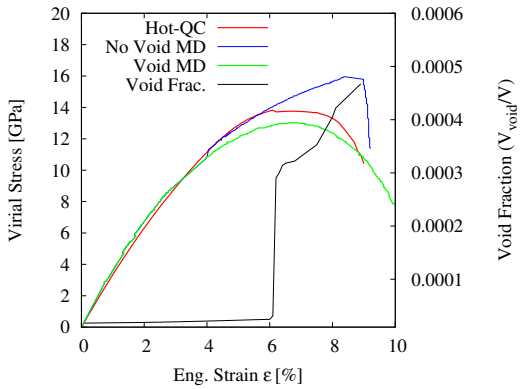

Figure 5: Virial stress for the triaxial loading case compared with MD results [14]. Note that at 6% of deformation the cavitation is reached and the material loss stiffness.

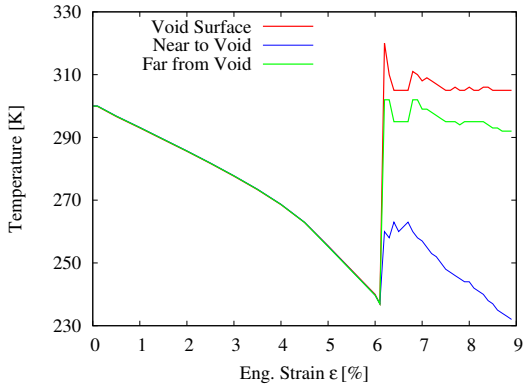

Figure 6: Temperature evolution during void growth process at different positions. Three temperatures are shows: a) void surface b) position close to the void surface and c) position away from the void surface.

pute a macroscopic response of the whole crystal, where fracture is clearly identified.

5 ACKNOWLEDGMENT

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