FINITE-TEMPERATURE SIMULATION OF NANOVOID GROWTH BY DISLOCATION EMISSION

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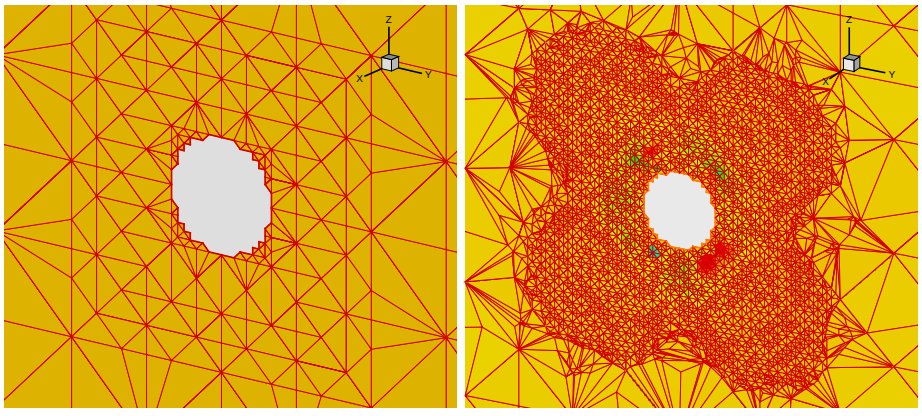
Summary Tensile failure of metals often occurs through void nucleation, growth and coalescence. In high-purity metals, void nucleation often operates at the nanoscale and is followed by plastic cavitation when the void attains the critical size for dislocation emission. This work is concerned with the study of plastic nanovoid cavitation in fcc crystals at finite temperature. In particular, the Quasicontinuum (QC) method, suitably extended to finite temperatures, is taken as the basis for the analysis. 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.

INTRODUCTION

Within the last decade, 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 [1]. 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 indicates that there is a growth threshold controlled by the stress required to nucleate dislocation activity. The time-scale for complete dynamic fracture ($0.1-1$ μs) 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 modeling provides an alternative to MD simulation, especially for this type of problems.

The Quasicontinuum method (QC) is a multiscale modeling scheme that seamlessly links continuum and atomistic descriptions. In this work we are going to use an extension of the static QC theory first developed by [2] and subsequently adapted by [3], to systems in thermodynamic equilibrium and non-equilibrium (HotQC) established in [4]. The HotQC method is based on Jaynes' principle of maximum entropy [5] and on variational mean-field theory in order to construct effective thermodynamic potentials for systems of atoms away from equilibrium. In particular, the temperature field is not required to be uniform but, contrariwise, it is allowed to take different values from atom to atom. In addition, [4] resort to [6] variational formulation of coupled transport problems in order to couple the non-equilibrium thermodynamic potentials to the heat equation. The chief advantage of the HotQC approach is that it entirely bypasses the need to track the thermal fluctuations of the atoms. In particular, the time steps required in calculations are set by the diffusional time scale, which is much greater than the time scale of the atomic vibrations.



(a) (b)

Figure 1. Close-ups of finite element mesh used in the QC reduction. a) Initial mesh, including a fully atomistic region around the void. b) Typical final mesh, showing mesh refinement resulting in an extended fully-atomistic region that encompasses all the dislocations emitted by the void.

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APPLICATIONS

In this work, we apply the HotQC method to the study of quasistatic void growth in copper single crystals at finite temperature under triaxial and uniaxial expansion. We specifically consider a cubic computational cell of 78 nm in size encompassing 216^3 unit cells and containing a total of 5.1×10^6 atoms. The boundary of the cell is aligned with the cube directions. A spherical 2.0 nm void is introduced at the center of the cell and full atomistic resolution is initially provided within a $8a \times 8a \times 8a$ region. Away from this fully-atomistic region, the initial triangulation is gradually coarsened with the result that the initial computational mesh contains 900 representative atoms only. The mesh is subsequently adapted so as to ensure that all dislocations are embedded within a sizeable atomistic region at all times [3] (see Fig. 1).
The computational cell is strained to 30% deformation by means of displacement control at its outer boundary. The initial temperatures and nominal strain rates under consideration range from 150K to 600K and from 2.5×10^5 s^{-1} to 2.5×10^{11} s^{-1}, respectively. The interatomic potential used in the calculations is Johnson's Embedded-Atom Method (EAM) potential [7]. The calculations characterize the dislocation structures and kinetics that mediate cavitation and the early stages of void growth, as well as the transient temperature fields attendant to the evolving dislocation structures.

CONCLUSIONS

We have applied an extension of the QC method to study the thermomechanical behavior of a nanovoid under tension. 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. The great advantage of HotQC is that it entirely bypasses the need to track the thermal fluctuations of the atoms in detail, a requirement that often besets molecular dynamics. In particular, the time steps required for the numerical solution of the problem are set by the diffusional time scale, which is much greater than the time scale of the atomic vibrations. In this manner, HotQC enables the tracking of diffusive processes over very long periods of time, while simultaneously building atomistic realism into the model.

References

[1] Seppala E.T., Belak J. and Rudd R.E.: *Physical Review B* **69**:134101, 2004.
[2] Tadmor E.B., Ortiz M. and Phillips R.: *Philos. Mag.* **73**:1529–1563, 1996.
[3] Knap J. and Ortiz M.: *J. Mech. Phys. Solids* **49**:1899–1923, 2001.
[4] Kulkarni Y., Knap J. and Ortiz M.: *J. Mech. Phys. Solids* **56**:1417–1449, 2008.
[5] Jaynes E.: *Physical Review Series II* **106**:620–630, 1957.
[6] Yang Q., Stainier L. and Ortiz M.: *J. Mech. Phys. Solids* **54**:401–424, 2006.
[7] Johnson R. A.: *Physical Review B* **37**:3924–3931, 1988.