Mechanics of Materials 90 (2015) 253–267

Contents lists available at ScienceDirect

Mechanics of Materials

journal homepage: www.elsevier.com/locate/mechmat

Finite-temperature non-equilibrium quasi-continuum analysis of nanovoid growth in copper at low and high strain rates

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ARTICLE INFO

Article history:
Received 14 August 2014
Received in revised form 14 January 2015
Available online 7 March 2015

Keywords:
Non-equilibrium statistical thermodynamics
Meanfield theory
Void growth
Nanovoids
Finite temperature

ABSTRACT

We study dynamic nanovoid growth in copper single crystals under prescribed volumetric strain rates ranging from moderate ($\dot{\epsilon} = 10^5\ s^{-1}$) to high ($\dot{\epsilon} = 10^{10}\ s^{-1}$). We gain access to lower strain rates by accounting for thermal vibrations in an entropic sense within the framework of maximum-entropy non-equilibrium statistical mechanics. We additionally account for heat conduction by means of empirical atomic-level kinetic laws. The resulting mean trajectories of the atoms are smooth and can be integrated implicitly using large time steps, greatly in excess of those required by molecular dynamics. We also gain access to large computational cells by means of spatial coarse-graining using the quasicontinuum method. On this basis, we identify a transition, somewhere between 10^7 and $10^8\ s^{-1}$, between two regimes: a quasistatic regime characterized by nearly isothermal behavior and low dislocation velocities; and a dynamic regime characterized by nearly adiabatic conditions and high dislocation velocities. We also elucidate the precise mechanisms underlying dislocation emission from the nanovoids during cavitation. We additionally investigate the sensitivity of the results of the analysis to the choice of interatomic potential by comparing two EAM-type potentials.

1. Introduction

The mechanisms of void nucleation, growth and coalescence are thought to mediate ductile failure and spallation of metals and, in that connection, have been the subject of extensive study. Under shock loading conditions, voids may nucleate at the nanoscale, e.g., by vacancy diffusion and aggregation (Reina et al., 2011). The resulting *nanovoids* subsequently grow by the emission of discrete lattice dislocations through a variety of intricate dislocation reaction paths (Marian et al., 2004, 2005; Meyers et al., 2009). At extremely high strain rates, nanovoid growth can be effectively simulated using molecular dynamics (Belak, 2002; Seppälä et al., 2004; Dávila et al., 2005; Traiviratana et al., 2007; Rudd, 2009; Bringa et al., 2010b; Lubarda, 2011; Tsuru and Shibutani, 2007). These studies reveal, among other useful insights, that nanovoids indeed cavitate upon the attainment of a critical stress or strain through the emission of shear and/or prismatic dislocation loops, resulting in irreversible void growth.

Despite its appeal, molecular dynamics suffers from a number of essential limitations. Foremost among these is the need to resolve every single thermal vibration of each atom in the computational sample, which restricts typical time steps to the femtosecond range. This restriction immediately places slow or long-term phenomena beyond the reach of molecular dynamics, thereby severely curtailing its scope. In particular, nanovoid growth under strain rates below $\sim 10^7\ s^{-1}$, which covers the vast majority of practical applications in engineering, cannot be studied

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http://dx.doi.org/10.1016/j.mechmat.2015.02.007
0167-6636/

by molecular dynamics. Additional difficulties arise in connection with the thermal and thermodynamical aspects of the simulations. Thus, molecular dynamics simulations are often carried out either in the microcanical or canonical ensemble, in the latter case by recourse to thermostating, Langevin dynamics and other techniques (cf., Andersen, 1980; Nosé, 1984; Hoover, 1985; Hünenberger, 2005; Bussi and Parrinello, 2008). However, these computational devices are *ad hoc* and often unrealistic and compromise the fidelity and predictiveness of the simulations. Not unrelated are the facts that molecular dynamics simulations tend to be noisy, which compounds the interpretation of results, especially as regards mesoscale phenomena such as the establishment and evolution of temperature fields, the role of heat transport and others. In particular, atomic-level noise in molecular dynamics simulations obscures lattice-level mechanisms such as dislocation reactions, especially at high strain rates. Finally, the study of defects at realistic concentrations, which are often in the parts per million, requires consideration of extremely large computational cells. Under these conditions, the explicit treatment of every atom in the cell is exceedingly wasteful, as only the cooperative behavior of large numbers of atoms—and not the behavior of individual ones—is of interest. This situation is strongly suggestive of the use of coarse-graining techniques, such as the quasicontinuum method (Tadmor et al., 1996), in order to weed out redundant and inconsequential degrees of freedom.

In this study, we overcome these difficulties by means of the finite-temperature quasicontinuum method (HotQC) of Kulkarni et al. (Kulkarni et al., 2008; Ariza et al., 2012; Ponga et al., 2012; Venturini et al., 2014). The aim of HotQC is to account for thermal effects, including atomic-level heat conduction, without the need for tracking every thermal vibration of the atoms. The approach is based on Jayne's *maximum entropy principle* (Jaynes, 1957a,b), which enables the statistical treatment of systems away from equilibrium. By maximizing a suitable constrained entropy, effective thermodynamic potentials are identified which characterize the instantaneous state of a system and supply driving forces for its evolution. However, unlike conventional equilibrium thermodynamic potentials such as the free energy, the new thermodynamic potentials are well-defined away from equilibrium, e.g., in the presence of strong temperature gradients. Under such conditions, HotQC characterizes the evolution of the system by means of *empirical* kinetic equations of the Onsager type (Onsager, 1931a,b; De Groot and Mazur, 1962). These kinetic relations may be regarded as an atomic-level *Fourier law* of heat conduction and, similarly to interatomic potentials, are subject to modeling. In practice, the exact evaluation of the requisite non-equilibrium thermodynamic potentials is generally intractable. However, they can be effectively approximated by means of variational meanfield theory and the resulting variational framework provides a convenient basis for the formulation of computationally tractable models, with or without spatial coase-graining. The fidelity of HotQC has been carefully assessed by Kulkarni et al. (2008) and Venturini et al. (2014) by direct comparison with experimental observation, including equilibrium properties of metallic alloys including lattice parameter, linear thermal expansion coefficient, elastic moduli and surface segregation concentration. Venturini et al. (2014) have additionally assessed the fidelity of empirical kinetic relations by means of two test cases: Heat conduction in silicon nanowires and hydrogen storage in palladium. In all cases, the ability of HotQC to properly account for equilibrium properties, structure-dependent transport properties and the long-term behavior of atomic systems over exceedingly long times is remarkable.

In the present work, whereas the thermal vibrations are accounted for in an entropic sense by recourse to max-ent, we account explicitly for microinertia, i.e., the dynamics attendant to void growth at the mesoscale. This consideration of mesoscale dynamics raises fundamental and long-standing issues of double counting for inertia, stability of time-stepping algorithms and phonon trapping resulting from spatial coarse-graining. Remarkably, the entropic treatment of thermal vibrations results in mean atomic trajectories that are slowly varying, or smooth, on the thermal time scale. In particular, the mean atomic trajectories are free of thermal vibrations, with the result that inertia is not double-counted. In addition, the smoothness of the mean atomic trajectories enables the use of implicit time-integration methods, such as Newmark's algorithm (Newmark, 1959), with exceedingly large time steps, in effect opening the way for the analysis of slow processes and the long-term behavior of atomistic systems. Finally, the smoothness of the mean atomic trajectories enables the introduction of spatial coarse-graining, e.g., by means of the quasicontinuum method, without spurious internal reflections and wave trapping at boundaries between regions of varying spatial resolution.

By this means, in the present paper we extend previous studies of dynamic nanovoid growth in copper single crystals (Seppälä et al., 2004; Dávila et al., 2005; Bringa et al., 2010b) to strain rates greatly below those accessible to molecular dynamics. We specifically study the effect of micro-inertia in nanovoids, with particular focus on mechanisms of dislocation emission, for strain rates ranging from moderate ($\dot{\epsilon} = 10^5\ s^{-1}$) to high ($\dot{\epsilon} = 10^{10}\ s^{-1}$). Another focus of the study concerns the role and extent of heat generation and conduction during dislocation emission. In this regard, HotQC conveniently affords clarity in the interpretation of calculation results by differentiating sharply between heat and temperature and mesoscopic dynamics. In particular, it supplies well-defined atomic-level temperature fields and their evolution. On this basis, we identify a transition, somewhere between 10^7 and $10^8\ s^{-1}$, between two regimes: a quasistatic regime characterized by nearly isothermal behavior and low dislocation velocities; and a dynamic regime characterized by nearly adiabatic conditions and high dislocation velocities. We additionally investigate the sensitivity of the results of the analysis to the choice of interatomic potential by comparing two EAM-type potentials by Mishin et al. (2001) and Johnson (1988).