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A closed-form criterion for dislocation emission in nano-porous materials under arbitrary thermomechanical loading

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Our traditional view of void nucleation is associated with interface debonding at second-phase particles. However, under extreme dynamic loading conditions second-phase particles may not necessarily be the dominant source of void nucleation sites. A few key experimental observations of laser spall surfaces support this assertion. Here, we describe an alternative mechanism to the traditional view, namely shock-induced vacancy generation and clustering followed by nanovoid growth mediated by dislocation emission. This mechanism only becomes active at very large stresses. It is therefore desirable to establish a closed-form criterion for the macroscopic stress required to activate dislocation emission in porous materials. Following an approach similar to Lubarda and co-workers, we derive the desired criterion by making use of stability arguments applied to the analytic solutions for the elastic interactions of dislocations and voids. Our analysis significantly extends that of Lubarda and co-workers by accounting for a more general stress state, finite porosity, surface tension, as well as temperature and pressure dependence. The resulting simple stress-based criterion is validated against a number of molecular dynamics simulations with favorable agreement.

1. Introduction and background

Failure of ductile metals has long been attributed to the microscopic processes of void nucleation, growth, and finally coalescence leading to fracture (McClintock, 1968; Rice and Tracey, 1969; Curran et al., 1987; Freund, 1990; Tvergaard, 1990). Some of the earliest investigations regarded void nucleation as a cavitation instability in an otherwise homogeneous elastic–perfectly plastic (Bishop et al., 1945; Hill, 1950), non-linear elastic (Ball, 1982), or power-law hardening medium (Huang et al., 1991). The more accepted view of void nucleation is that it occurs at some material defects. Traditionally, these void nucleating material defects have been associated with second-phase particles (Le Roy et al., 1981; Needleman, 1987). For example, hard inclusions, such as carbide and oxide particles, may either crack or debond from the ductile metal matrix, see Lindley et al. (1970), Argon et al. (1975), and Beremin (1981). Voids have also been seen to nucleate within soft inclusions, e.g. sulfides (Benzerga et al., 2004). However, much of this understanding of void nucleation at second-phase particles has been gleaned from observations of quasi-static fracture surfaces. At high enough tensile stresses, e.g. levels achievable in

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laser shock experiments and related applications, second-phase particles may not necessarily be the dominant source of void nucleating material defects, and the recent observations of Pedrazas et al. (2012) seem to support this assertion.

A number of investigators have hypothesized the existence of nanoscale voids (on the order of 1 nm in size) in shocked metals, see for example Lubarda et al. (2004), Tang et al. (2011), Reina et al. (2011), and Wilkerson and Ramesh (2014). Vacancy clustering is one potential mechanism for the formation of these nanovoids. Reina et al. (2011) made use of lattice kinetic Monte Carlo simulations to demonstrate that the timescales associated with this process are in fact feasible (see Section 2). Assuming the existence of these nanovoids, numerous atomistic studies have computed the level of tensile stress ($\sim \mu/10$) required to effectively grow these voids by emitting dislocation loops from the void surface (Belak, 1998; Rudd and Belak, 2002; Seppälä et al., 2004; Traiviratana et al., 2008; Meyers et al., 2009; Bringa et al., 2010; Tang et al., 2011; Ariza et al., 2012). These levels of tensile stresses ($\sim \mu/10$) have been achieved in a number of laser shock experiments, e.g. Moshe et al. (2000), Cuq-Lelandais et al. (2009), and Pedrazas et al. (2012), implying that such dislocation emission may be an important mechanism of void growth at these extreme loading rates. Given the potential importance of this mechanism, it is desirable to establish a closed-form criterion for the macroscopic stress required for dislocation emission in porous materials.

Through a simple dislocation analysis, Lubarda et al. (2004) derived such a closed-form criterion for the critical far-field hydrostatic stress required to cause the emission of a straight edge dislocation from an infinitely extended cylindrical void in an otherwise homogeneous, linearly elastic, isotropic infinite medium. Although this analysis does not capture the actual geometry associated with the physical problem of interest, i.e. dislocation loops emitted from a spherical void in an anisotropic medium, favorable comparisons with atomistic simulations demonstrated the utility of such an analysis. Recently, Lubarda (2011a) extended this analysis to account for a far-field biaxial stress state. In order to make the criterion more useful for the continuum level prediction of dynamic ductile failure, we provide a number of further extensions to the analysis of Lubarda (2011a) accounting for the following:

- a general three-dimensional macroscopic stress state
- a distribution of void sizes
- finite porosity
- surface tension
- temperature dependence
- hydrostatic pressure dependence.

The present paper is organized as follows. Section 2 provides further motivation for the role of vacancy clustering and subsequent dislocation emission in the dynamic failure of metals at extreme strain rates ($\gtrsim 10^6\ \mathrm{s}^{-1}$). In Section 3, we approximate the stress fields and Peach–Koehler forces experienced by a dislocation near a void surface in a porous material. Here the porous material is composed of a particular void size distribution $g(a)$ with an associated finite porosity φ, and is subject to a general three-dimensional stress state $\mathbf{\Sigma}$. Our strategy involves the construction of an auxiliary problem associated with this physical problem, but simple enough to permit analytical solutions. These Peach–Koehler forces are then utilized in Section 4 to establish a criterion for dislocation emission based on the stability arguments first proposed by Rice and Thomson (1974) (placed in a somewhat more physical context here). Section 4 also provides a rather detailed discussion of the role of various parameters and physics on the criterion for dislocation emission. In Section 5 we provide a fairly extensive validation of the emission criteria against molecular dynamics predictions of dislocation emission under various stress states and geometries. In addition to the validation effort, we provide a strategy for approximately calibrating the dislocation emission criterion parameters against atomistic calculations of homogeneous dislocation nucleation. Lastly, a

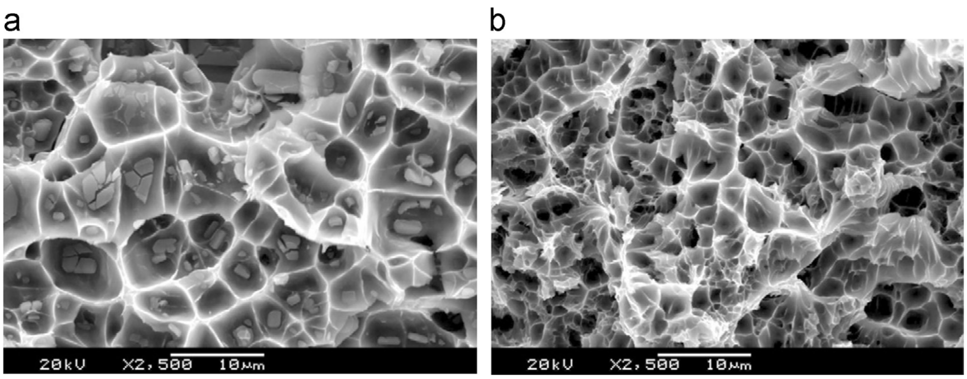

Fig. 1. SEM images of spall fracture surfaces reported in Pedrazas et al. (2012) for (a) 99% commercially pure aluminum and (b) 99.999% high-purity aluminum. Most of the voids in the commercially pure aluminum shown in (a) nucleate from second-phase particles, e.g. Al_3Fe, whereas for the high-purity aluminum only a very small fraction of the dimples (~5%) contained second-phase particles, implying that the bulk of these voids nucleate by an alternative mechanism, e.g. vacancy clustering and subsequent growth by dislocation emission.