Acta Materialia 101 (2015) 40–47

Contents lists available at ScienceDirect

Acta Materialia

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

Capturing the effects of free surfaces on void strengthening with dislocation dynamics

Joshua C. Crone *, Lynn B. Munday, Jaroslaw Knap

U.S. Army Research Laboratory, Aberdeen Proving Ground, MD 21005, USA

ARTICLE INFO

Article history:
Received 24 July 2015
Revised 25 August 2015
Accepted 28 August 2015

Keywords:
Discrete dislocation dynamics
Void strengthening
Surface effects

ABSTRACT

Void strengthening in crystalline materials refers to the increase in yield stress due to the impediment of dislocation motion by voids. Dislocation dynamics (DD) is a modeling method well suited to capture the physics, length scales, and time scales associated with void strengthening. However, previous DD simulation of dislocation–void interactions have been unable to accurately account for the strong image forces acting on the dislocation due to the void's free surface. In this article, we employ a finite-element-based DD method to determine the obstacle strength of voids, defined as the critical resolved shear stress for a dislocation to glide past an array of voids. Our results demonstrate that the attractive image forces between the dislocation and free surface significantly reduce the obstacle strength of voids. Effects of surface mobility and stress concentrations around the void are also explored and are shown to have minimal effect on the critical stress. Finally, a new model relating void size and spacing to obstacle strength is proposed.

Published by Elsevier Ltd. on behalf of Acta Materialia Inc.

1. Introduction

The plastic deformation of crystalline materials is primarily governed by the evolution of dislocations. Interactions of dislocations with atomic defects and microstructural features are known to significantly affect dislocation motion, altering the macroscopic mechanical response. Voids, frequently introduced during processing, additive manufacturing, or irradiation, are one such feature that has been found experimentally to increase yield strength with increasing void density [1,2]. The increased yield strength is primarily attributed to the pinning of dislocations at the voids [2]. Consequently, the strength of crystalline material is dependent on the obstacle strength of the void configuration, defined as the magnitude of stress necessary for a dislocation to bypass a void array. Despite the fundamental importance of the above void-strengthening in determining the material response in porous crystals, few accurate models exist.

Several studies of the interaction of dislocations and voids have been carried out by means of molecular dynamics (MD) [3–8]. These studies have provided tremendous insight into bypass mechanisms at the atomic scale, such as glide [3], climb [4], and inertial effects [7]. However, void sizes directly accessible to MD are typically in the range of 1–6 nm, whereas corresponding void sizes found in crystalline materials commonly range from tens of nanometers to microns [9–13]. Furthermore, MD, due to its limitations in the size of the computational domain, can frequently only be applied to modeling a single void in a periodic array of voids. Such an idealized arrangement of voids is unlikely to provide a statistically representative characterization of plasticity in crystals with porosity. Finally, temporal scales characteristic to MD require strain rates on the order of 10^6–10^9 1/s, well outside of the range encountered in typical applications.

In contrast with MD, dislocation dynamics (DD) is a more suitable choice for studying yield strength and early stages of strain hardening at larger length and time scales. DD has been shown capable of capturing the strengthening mechanisms due to interaction of dislocations with other defects [14–16]. However, modeling of voids by means of DD has been challenging due to the need to account for the presence of surfaces. Orowan [17] was the first to explicitly model the interaction of dislocations with other defects, namely impenetrable inclusions where free surfaces are not applicable. Subsequently, Bacon, Kocks, and Scattergood [18] expanded Orowan's model to incorporate dislocation self-interactions. According to this model, the critical resolved shear stress, τ_c, required for an edge dislocation to bypass a periodic array of impenetrable inclusions is given by

$$\tau_c = \frac{\mu b}{2\pi L}\left[\ln\left(\frac{\overline{D}}{b}\right) + \Delta\right] \qquad (1)$$

* Corresponding author.
E-mail address: joshua.crone.civ@mail.mil (J.C. Crone).

http://dx.doi.org/10.1016/j.actamat.2015.08.067
1359-6454/Published by Elsevier Ltd. on behalf of Acta Materialia Inc.

where μ is the shear modulus, b the magnitude of the Burgers vector, D the void diameter, L the void spacing, $\overline{D} = (D^{-1} + L^{-1})^{-1}$, and $\Delta = 0.7$. Scattergood and Bacon [19] extended this model further, replacing impenetrable inclusions with voids. Their model yielded the same functional form of Eq. (1), albeit with $\Delta = 1.52$. At present, the model of Scattergood and Bacon is widely accepted for modeling of the obstacle strength of voids. However, Scattergood and Bacon openly discuss a number of significant simplifications in their model. First and foremost, the image forces which account for the interaction between the dislocation and the free surface are only accounted for at the dislocation-surface intersection point and are neglected otherwise. Furthermore, the effect of the free surface is approximated by means of the simplified geometry of a half-space. In addition, the applied stress field is assumed to be uniform, ignoring the effect of stress concentrations. Finally, mobility of the dislocation along the void's free surface is modified via a surface energy term without a systematic study of its effect on τ_c.

Before DD can be reliably applied to study large scale void-strengthening effects at high void and dislocation densities, it is important to accurately model the obstacle strength of voids in idealized geometries, such as a periodic array. Therefore, the focus of this article is twofold. First, we re-examine the approximations made by Scattergood and Bacon [19] and determine their effects on τ_c. The development of advanced computational tools for computing image forces with arbitrary geometries [20,21] enables us to improve upon these previous predictions with more accurate treatment of image forces. An understanding of the various approximations is a critical step towards performing large scale studies that are both physically accurate and computationally tractable. Second, using a more accurate treatment of the surface effects, we present a new model for the obstacle strength of voids.

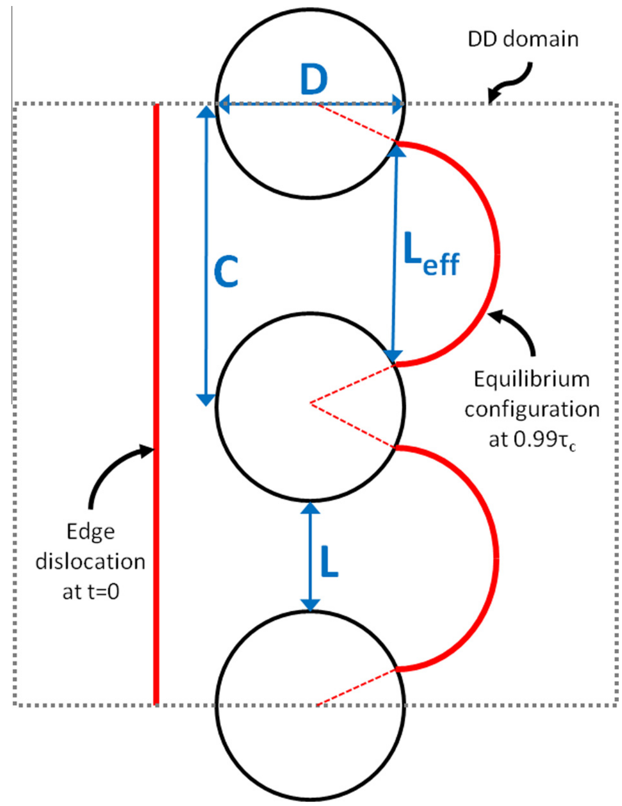

Fig. 1. Schematic of the simulation model setup. Virtual segments are represented by the dotted lines connecting the dislocation line to the center of the voids.

2. Methodology

2.1. Simulation procedure

Modeling of dislocation dynamics (DD) with surface effects is performed by coupling a finite element method (FEM) solver [20,21] to the ParaDiS DD simulator [22] following the methodology of van der Giessen and Needleman [23]. A detailed description of the DD and FEM algorithms can be found in Refs. [22,20], respectively. We briefly discuss the main features specific to modeling dislocation–void interactions.

The focus of this work is to identify the minimum resolved shear stress (τ_c) required for a dislocation to bypass a periodic array of voids. To this end, we follow the model setup of Scattergood and Bacon [19], shown in Fig. 1, where an infinite straight edge dislocation is placed near a 1D array of voids. A shear stress (σ_{xy}^{ext}) is applied to drive the dislocation towards the void array. If an equilibrium configuration exists in which the dislocation remains attached to the void, σ_{xy}^{ext} is increased until the dislocation breaks away and bypasses the void array. τ_c is determined when the value of the σ_{xy}^{ext} to bypass the voids is within 1% of the stress to achieve equilibrium. We assume that a static equilibrium has been reached when the peak of the bowed-out dislocation line has not advanced for at least 10^4 time steps. Simulations with a stricter criteria requiring no advancement for 10^5 time steps show no effect on τ_c.

Peach–Koehler forces are computed on each dislocation segment. The forces include contributions from the externally applied stress (f^{ext}), image stress (f^{img}), and the stress due to all dislocation segments in the system (f^{disl}). The calculation of f^{ext} in previous DD simulations with voids have assumed only a uniform applied stress field [19]. However, under an applied stress, stress concentrations occur around the void and alter the local stress field. In order to determine the effect of these stress concentrations, we compare the results of τ_c using a uniform applied stress to the results explicitly including the stress concentrations. The computation of f^{disl} is performed in ParaDiS using the non-singular dislocation stress field [24] with a core radius of 1b.

Image forces are required due to the presence of voids and the resulting deviation of dislocation stress field from that in an infinite body. Enforcement of traction free boundary conditions on the surfaces and solving the resulting linear elastic boundary value problem (BVP) provides the corrective image stress field. The image stress is then superimposed with the stress field due to the dislocations in an infinite body [23]. Conservation of the Burgers vector is assured by the introduction of virtual segments [25,20] extending from the surface-piercing dislocations to the center of the void [26] (c.f Fig. 1).

In order to avoid the high computational expense of numerically calculating the image stress field, analytic solutions for the image stress and resulting image force have been developed for some simple geometries. For example, a solution for a straight, semi-infinite dislocation piercing the free surface of a half space was introduced by Lothe [27]. This solution yields a particularly simple dislocation equilibrium condition [19]

$$E\cos(\theta) - E'\sin(\theta) = 0 \tag{2}$$

where E is the strain energy per unit length of a dislocation, θ is the angle between the dislocation line and the free surface as shown in Fig. 2, and $E' = \partial E/\partial\theta$ is the orientation derivative of E. In Fig. 2b, we illustrate how the left hand side of Eq. (2) can be used to approximate the image forces acting on the dislocation at the surface-dislocation intersection point. Further details on how the Lothe equation is employed to approximate the image forces from a void