International Journal of Plasticity 27 (2011) 1055–1071

Contents lists available at ScienceDirect

International Journal of Plasticity

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

Investigations of pipe-diffusion-based dislocation climb by discrete dislocation dynamics

Y. Gao, Z. Zhuang *, Z.L. Liu, X.C. You, X.C. Zhao, Z.H. Zhang

Applied Mechanics Lab., Dept. of Engineering Mechanics, School of Aerospace, Tsinghua University, Beijing 100084, China

ARTICLE INFO

Article history:
Received 1 March 2010
Received in final revised form 11 October 2010
Available online 19 November 2010

Keywords:
Dislocation dynamics
Dislocation climb
Pipe diffusion
Prismatic loops
Dislocation dipole

ABSTRACT

A new numerical dislocation climb model based on incorporating the pipe diffusion theory (PDT) of vacancies with 3D discrete dislocation dynamics (DDD) is developed. In this model we hold that the climb rate of dislocations is determined by the gradient of the vacancy concentration on the segment, but not by the mechanical climb force as traditionally believed. The nodal forces on discrete dislocation segments in DDD simulation are transferred to PDT to calculate the vacancy concentration gradient. This transfer establishes a bridge connecting the DDD and PDT. The model is highly efficient and accurate. As verifications, two typical climb-involved examples are predicted, e.g. the activation of a Bardeen–Herring source as well as the shrinkage and annihilation of prismatic loops. Finally, the model is applied to study the breakup process of an infinite edge dislocation dipole into prismatic loops. This coupling methodology provides us a useful tool to intensively study the evolution of dislocation microstructures at high temperatures.

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1. Introduction

Diffusion-controlled dislocation climb is a non-conservative motion that occurs by absorbing or emitting point defects from or into dislocations. This kind of dislocation motion exerts a significant influence on crystal plastic behavior at high temperatures (Allnatt and Lidiard, 1993; Berry et al., 2006; Caillard and Martin, 2003; Chen et al., 2010; Hirth and Lothe, 1982; Xiang and Srolovitz, 2006). Many groups have introduced the climb mechanism into constitutive laws (Fedelich, 2002; Hartmaier et al., 2003; Hiratani et al., 2003; Lebensohna et al., 2010; Li et al., 2009; Pontes et al., 2006). However, phenomenological approaches are insufficient to reveal the intrinsic mechanism for the dislocation climb process. Discrete dislocation dynamics (DDD), as an effective computational technique to simulate the dislocation motions, plays an important role in studying how the dislocation microstructure affects the mechanical properties of metals, such as size effect (Akarapu et al., 2010; Deshpande et al., 2005; Weygand et al., 2008), strain hardening (Bulatov et al., 2006; Devincre et al., 2008), multiphase interface plasticity (Yashiro et al., 2006), impact property (Shehadeh et al., 2005), fracture (Van der Giessen et al., 2001), fatigue (Shin et al., 2005), friction (Deshpande et al., 2004), etc. However, to our best knowledge, the technique for studying the dislocation climb process by coupling the DDD with the diffusion theory of point defects has been rarely documented (Mordehai et al., 2008; Raabe, 1998). A vast majority of the DDD simulations either took no considerations to dislocation climb or treated climb as a conservative motion, i.e. with a constant drag coefficient similar to glide process.

For instance, several groups introduced dislocation climb into 2D-DDD simulations by assuming a proportional dependency between the climb force and the climb rate (Argaman et al., 2001a,b; Hartmaier et al., 2005). Amodeo and Ghoniem (1990) adopted a phenomenological assumption that the climb velocity is a function of the applied stress and temperature

* Corresponding author. Tel./fax: +86 10 62783014.
E-mail address: zhuangz@tsinghua.edu.cn (Z. Zhuang).

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doi:10.1016/j.ijplas.2010.11.003