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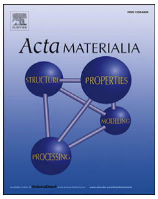

Full length article

Annihilation of edge dislocation loops via climb during nanoindentation

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A R T I C L E I N F O

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A B S T R A C T

In this work, we explore the role of dislocation climb in annihilating the dislocation microstructure produced during a nanoindentation test. We produce creep conditions in Molecular Dynamics (MD) simulations of nanoindentation and show that half prismatic edge dislocation loops annihilate via pipe diffusion of vacancies from the free surface. Inspired by the MD simulations, we develop a model for the annihilation rate of these loops via pipe diffusion and compare it with the contribution of bulk diffusion. The model allows us discussing the temperatures at which we expect climb to prevail in experimental conditions and explain why climb is imperative during nanoindentation experiments.

1. Introduction

Nanoindentation is a widely used technique to study mechanical properties of materials on the nanoscale. In this experimental technique, a tip is pushed into a material and deforms it plastically [1,2]. While traditionally the mechanical response is employed to calculate the hardness and elastic modulus, there is an increasing interest in using this type of experiment to measure other mechanical properties such as hardening exponent, creep parameters, residual stresses and to understand plasticity on the nanoscale [3–11]. Therefore, it is essential to understand the various dislocation mechanisms acting beneath the indenter in order to interpret the measured mechanical response. At room temperature, it is common to consider mainly dislocation nucleation and glide [12–23]. For instance, in the popular Nix-Gao Model [24], it is assumed that prismatic loops are nucleated in order to fulfill the geometrical constraints of the indentation, so that the dislocation density in the plastic zone corresponds to the volume pushed by the tip.

However, the thermal energy during the indentation is influencing additional dislocation mechanisms. In addition to nucleation and glide of dislocations, thermally activated mechanisms are operating within the plastic zone. The role of these processes is even more important in nanoindentation experiments at high temperatures, which became increasingly frequent in recent years [8,9,25]. One possible thermally activated dislocation mechanism is the cross-slip of screw dislocations inside the plastic zone. This mechanism allows screw dislocations to change slip planes and consequently part of the dislocation microstructure annihilates. However, prismatic dislocation loops, full and half, are formed during indentation [14,26]. The full prismatic loops move into the material away from the indent (out-of-plane direction) and the half prismatic loops with two ends touching the upper/free surface move in parallel to the top surface (in-plane direction). These dislocations, which are of edge character, can not be annihilated via cross-slip but by climb; the edge dislocation loops shrink by absorbing vacancies. This motion is also thermally activated and involves the diffusion of vacancies both from the bulk (bulk diffusion) or through the dislocation core (pipe diffusion) [27–31].

The importance of dislocation climb to deformation creep is well known [32–35]. However, its contribution to nanoindentation is not well explored, although some evidence for its importance can be found in literature. Phani and Oliver [25] recently performed high temperature nanoindentation creep experiments. Upon exploring the effect of the indenter size, strain rate and temperature on hardness, they pointed out that temperature effect is dominant, especially at high temperatures. In order to quantitatively relate between the strain rates and stresses during nanoindentation, they considered an effective diffusion coefficient which combined both bulk self diffusion coefficient and the pipe

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diffusion coefficient [36]. This observation emphasizes that dislocation climb may be an important mechanism in nanoindentation experiments, especially at high temperatures.

In this work we explore the contribution of dislocation climb to the annihilation of the dislocation microstructure beneath the indent. We first employ molecular dynamics (MD) simulations to demonstrate the disappearance of the edge dislocation prismatic loops via dislocation climb, with an emphasis on the in-plane half prismatic loops. Inspired by the MD simulation results, a climb model for the annihilation of the in-plane half prismatic loops is presented. Based on the model, the contributions to the annihilation rate of pipe diffusion of vacancies from the upper surface and bulk diffusion is discussed.

2. Molecular dynamics simulations

2.1. Computational method

In order to demonstrate the importance of climb during nanoindentation, a model setup is constructed as shown schematically in Fig. 1a. A face centered cubic (FCC) Au thin film is first indented in MD simulations in order to generate a dislocation structure around the indent, followed by heating the system to stimulate annihilation of the dislocation structure via thermally activated processes. The thin film is indented by a spherical virtual indenter of radius 3.6 nm on its (111) surface. The bottom layer of atoms is fixed in the [111] crystallographic orientation (*z* axis) and the film is periodic in $[\bar{1}\bar{1}2]$ (*x*) and $[1\bar{1}0]$ (*y*) crystallographic orientations. The system's periodicity is 30 nm in each direction. The thin film height is 15 nm. The embedded-atom method (EAM) interatomic potential, with the parametrization proposed by Grochola et al. [37] for Au, is employed. A static relaxation by conjugate gradient followed by a relaxation via 30,000 MD time steps is performed. The time step during the dynamic parts is set to 3 fs. The indenter is then lowered into the film at a constant rate of 0.01 nm ps^{-1}, up to a depth equal to 3.36 nm. Once reaching the maximum depth, the indentation stops and the indenter is kept at a constant height through the rest of the simulation. The system is heated up to several targeted temperatures below the melting point, using the Nosé-Hoover thermostat during 100,000 MD time steps. In combination with the Parrinello-Rahman barostat, the volume is allowed to change so that the global pressures P_{xx} and P_{yy} are not nullified but kept at their values as obtained right at the end of indentation. This ensures that the thermal expansion is allowed but the internal stresses due to the indentation do not relax. During the last two stages, replicas of the system are quenched periodically via conjugate gradient. The quenched system is employed to identify and visualize the dislocation structures via the common neighbor analysis [38–40].

2.2. Simulation results

Before heating, the indentation generated a complex dislocation microstructure within the thin film (see Fig. 1b). The dislocation structure is composed of dislocation lines of various characters. For instance, dislocations with Burgers vectors parallel to upper surface

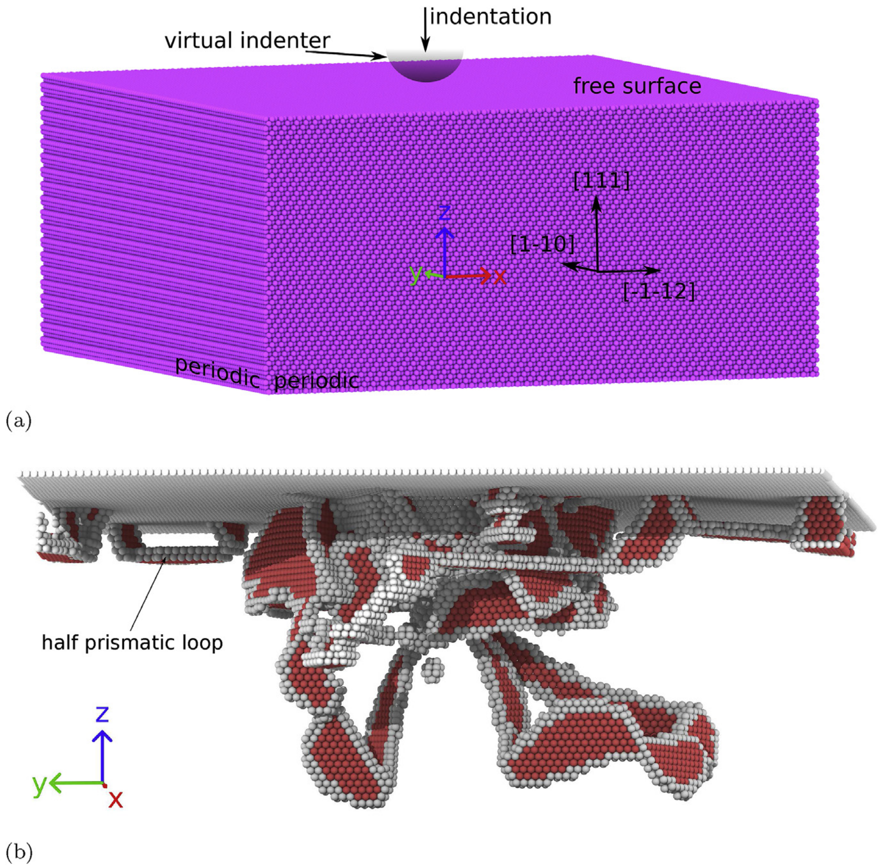

Fig. 1. (a) A schematic description of the atomistic model. The indentation is performed along the $[\bar{1}\bar{1}\bar{1}]$ crystallographic orientation while the film is periodic in the $[\bar{1}\bar{1}2]$ and $[1\bar{1}0]$ directions. (b) The dislocation microstructure at the end of indentation (indentation depth of 3.36 nm). Two in-plane prismatic half loops are clearly visible and a full prismatic loop in the out-of-plane direction is about to form. This final state is taken as the model dislocation microstructure before heating.