Journal of Nuclear Materials 508 (2018) 481–487

Contents lists available at ScienceDirect

Journal of Nuclear Materials

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

Impact of a dense helium-bubble superlattice on the deformation of copper by twinning

Ian S. Winter [a, *], Zhang-Jie Wang [b, c], Peter Hosemann [b], D.C. Chrzan [a]

[a] Department of Materials Science and Engineering, University of California, Berkeley, CA, 94720, USA
[b] Department of Nuclear Engineering, University of California, Berkeley, CA, 94720, USA
[c] Center for Advancing Materials Performance from the Nanoscale (CAMP-Nano) & Hysitron Applied Research Center in China (HARCC), State Key Laboratory for Mechanical Behavior of Materials, Xi'an Jiaotong University, Xi'an, 710049, China

ARTICLE INFO

Article history:
Received 4 August 2017
Received in revised form
16 February 2018
Accepted 24 May 2018
Available online 28 May 2018

ABSTRACT

Recent experimental work on helium-irradiated single-crystal (SC) and nano-twinned (NT) copper has shown that the formation of a helium bubble superlattice has a dramatic effect on the critical resolved shear stress of twin formation in SC copper pillars and twin migration in NT copper pillars. The mechanisms governing this dramatic change in the mechanical response of the material after helium irradiation are explained theoretically in this work. Atomistic simulations show that the presence of a helium bubble superlattice has a profound effect on twin nucleation and propagation, which are related to the mechanical responses of SC and NT copper respectively. Based on the simulations, we estimate that the bubble lattice can decrease the ideal twin nucleation stress compared to pure copper by approximately 50%. The modeled response of a step in a twin boundary to an applied shear stress leads to an increase in the critical resolved shear stress due to the bubble lattice. The computed increase is in qualitative agreement with experimental findings for NT copper.

© 2018 Published by Elsevier B.V.

1. Introduction

Experimental studies of face-centered cubic (FCC) materials reveal the formation of a He gas-bubble superlattice after heavy He-ion irradiation [1–3] at moderate temperatures (below $0.35T_m$). These bubble superlattices have a clear orientation relationship with the host matrix, and in the case of copper, the FCC bubble lattice constant, a_l, and bubble radius, r, are found to be approximately 7 nm and 1 nm respectively. Over the past four decades, however, little new information has been obtained regarding the effects on the mechanical properties of these superlattices. Recent work by Wang et al. has examined the effect of a He gas-bubble superlattice on the mechanical response of single-crystal (SC) and nano-twinned (NT) copper [4]. These experiments showed that (1) twin boundary migration appeared to preserve the gas-bubble superlattice while ordinary dislocation plasticity did not, and (2) that the gas-bubble superlattice greatly increased the critical resolved shear stress (CRSS) associated with twin boundary migration (a dominant deformation mechanism for the NT specimens), with the CRSS going from approximately 150 MPa for pure NT Cu to 350 MPa after He-ion irradiation of 2×10^{17} ions/cm^2. The increase in CRSS was shown to be within the same order of magnitude as the increase in CRSS predicted by the Friedel-Kroupa-Hirsch model (FKH) [5–7] after samples were aged for two weeks, presumably allowing the bubbles to equilibrate. This suggests that the change in CRSS is a result of a mechanism similar to precipitation hardening. Interestingly, compression tests of SC Cu (in which twin boundary migration would not be considered as a plastic deformation mechanism) showed a decrease in CRSS as a result of He-ion irradiation.

We employ atomistic simulations on He gas-bubble superlattices in FCC Cu in order to better understand the underlying mechanisms responsible for the change in CRSS by a gas-bubble superlattice. The gas-bubble superlattice's effect on the CRSS is examined both with respect to twin nucleation (for the case of SC Cu) and twin propagation (for the case of NT Cu). In both cases, a dramatic difference in the mechanical response of the gas-bubble superlattice is seen depending on the size of the helium bubble. In the case of twin nucleation, the strength of the material appears to be inversely related to helium bubble radius, as seen from both

* Corresponding author.
E-mail address: ian.winter@berkeley.edu (I.S. Winter).

https://doi.org/10.1016/j.jnucmat.2018.05.056
0022-3115/© 2018 Published by Elsevier B.V.

shear strength and stacking fault energy calculations. Twin propagation is examined by calculating the response of a stepped twin boundary to a pure shear stress. The results of this study show agreement with the experiment. Further, the FKH model appears to be applicable to the mechanical response of relatively small helium bubble radii ($r \leq 8$ Å) for this particular setup, but breaks down for larger bubbles.

2. Twin nucleation

It is possible that a change in twin nucleation behavior can describe the effect of bubble size on strength. Accordingly, molecular dynamics simulations were run in order to determine the effect of the bubble radius on the shear strength of the material, as this is a relatively simple calculation that can quickly gauge the effects of bubbles on the upper limit of strength. In conjunction with these simulations, static stacking fault energy calculations were carried out on a FCC void superlattice embedded in a Cu matrix.

Twin nucleation calculations were performed with an embedded atom method potential (EAM) developed by Mishin et al. [8] using the molecular dynamics code LAMMPS [9]. The Beck potential was used for He-He interactions [10]. With respect to Cu-He interactions, a Lennard-Jones potential of the form $V(r) = \varepsilon\left(\frac{\sigma}{r}\right)^{12}$ was developed, which captures only the repulsive interaction between Cu and He. The parameters for the Lennard-Jones potential were $\varepsilon = 5.52$ meV and $\sigma = 2.43$ Å. The shear strength (SS) simulations were performed following the approach of Iskandarov et al. [11]. A simulation cell with periodic boundary conditions was constructed and contained approximately 100,000 atoms. The supercell lattice vectors were oriented along $[11\bar{2}]$, $[1\bar{1}0]$, and $[111]$ respectively. The gas-bubble superlattice was constructed by superimposing an FCC superlattice on the Cu matrix and removing all Cu atoms within a given radius of superimposed lattice points, and adding He atoms such that the concentration of He in the bubbles was 1 He/vacancy site, which is roughly the same concentration as that calculated for equilibrium He bubbles in Fe [12]. The gas-bubble superlattice was defined such that the helium bubbles were of radius 5 Å or 10 Å and the nearest neighbor distance (center of bubble to center of bubble, $\frac{\sqrt{2}}{2}a_l$) 33.2 Å, which is approximately equal to the nearest neighbor distance of 30 Å measured by Wang et al. [4]. An increasing shear stress along $[11\bar{2}]$ direction was applied at a rate of 2.5 MPa/ps allowing all other stress components to relax while maintaining a temperature of 300 K. The $[11\bar{2}]$ direction was chosen as it is the weakest orientation in FCC Cu [13].

Stacking fault energy calculations were carried out in accordance with the work of Ogata et al. [14]. The calculations were performed for both pure FCC Cu, as well as Cu with a void superlattice of radius 5 Å and 10 Å (instead of helium bubbles for simplicity) at 0 K. Stacking fault energies were obtained by initially shifting neighboring (111) planes relative to one anther from 0 to b_{twin}, the Burgers vector of the leading partial dislocation, along the $[11\bar{2}]$ direction in order to form a stacking fault. This was then repeated along adjacent (111) planes in order to form a twin nucleus as shown in Fig. 1. The following stacking fault energies were calculated: γ_{US}, the stacking fault nucleation barrier (the first maximum value); γ_{ISF}, the stacking fault energy; γ_{UT}, twin nucleation barrier; as well as γ_{TBF}, the twin boundary formation energy.

Calculations were performed to determine how these parameters change with relation to the distance of the twin boundaries from the center of a bubble. A stacking fault was placed at the center of a row of bubbles on the (111) plane. The twin nucleation barrier as well as the twin stacking fault energy were calculated for twin nuclei of varying number of layers, with the center of the nucleus cutting through the middle of a bubble row. The twin boundary migration energy (TBME), the energy barrier to the migration of the twin, was defined as the difference between the twin nucleation barrier (local maximum) and the twin boundary formation energy (local minimum) [15].

$$\gamma_{TBME} = \gamma_{UT} - 2\gamma_{TBF}. \tag{1}$$

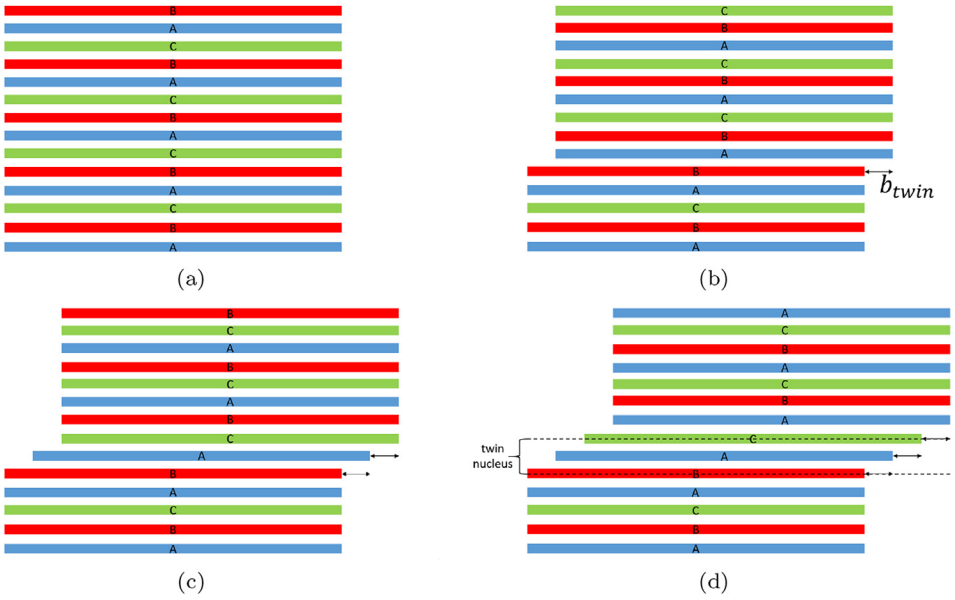

Fig. 1. Diagram representing the stacking fault energy calculations. Fig. 1a represents a set of (111) FCC planes with the ABC stacking. By shifting one section of planes over another by b_{twin} a stacking fault is formed, as shown in Fig. 1b. Repeating this procedure twice on higher planes (Fig. 1c and d) results in the formation of a twin nucleus (1d), which is bounded by HCP planes; those planes with ABA and ACA stacking.

Download English Version:

https://daneshyari.com/en/article/7962981

Download Persian Version:

https://daneshyari.com/article/7962981

Daneshyari.com