Acta Materialia 113 (2016) 194–205

Contents lists available at ScienceDirect

Acta Materialia

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

Full length article

Manipulating dislocation nucleation and shear resistance of bimetal interfaces by atomic steps

R.F. Zhang [a, *], I.J. Beyerlein [b], S.J. Zheng [c], S.H. Zhang [a], A. Stukowski [d], T.C. Germann [b]

[a] School of Materials Science and Engineering, and International Research Institute for Multidisciplinary Science, Beihang University, Beijing, 100191, China
[b] Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM, 87545, USA
[c] Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences, Shenyang, 110016, China
[d] Technische Universität Darmstadt, Jovanka-Bontschits-Str. 2, 64287, Darmstadt, Germany

ARTICLE INFO

Article history:
Received 13 March 2016
Received in revised form
7 May 2016
Accepted 7 May 2016

Keywords:
MD simulations
Interface
Dislocation
Plasticity
Mechanical strength

ABSTRACT

By means of atomistic simulations and interface dislocation theory, the mechanism of dislocation nucleation and shear resistance of various stepped fcc/bcc interfaces are comparatively studied using the Kurdjumov-Sachs (KS) Cu/Nb interface as a prototype. It is found that the introduction of atomic steps at the flat Cu{111}/{110}Nb KS interface does not change the most preferred slip systems, but influences the nucleation sites at the interface during tension loading, indicating that the flat and stepped interfaces possesses comparable energetic barriers for dislocation nucleation. During shear loading, the steps may significantly enhance the resistance to interface sliding by propagating partial dislocations that facilitate the emission and growth of parallel twins via cross slip. When the parallel twins are not favored or are hindered, the interface sliding will dominate in a "climbing peak-to-valley" manner. These results provide an effective pathway to solve the trade-off dilemma between dislocation nucleation and interface sliding by appropriately manipulating atomic steps at the flat interface in the design of high-strength metallic materials.

1. Introduction

Interfaces are central to the understanding of plastic deformation and mechanical strength in nanocomposites and heterostructures, as well as the control of their performance under extreme conditions. Interface-initiated plastic deformation in nanocomposites and heterostructures mainly involves two competing mechanisms, namely dislocation nucleation at the interface and interfacial sliding under shear. Both of these are closely correlated to the character of various defects at semicoherent or incoherent interfaces [1–16]. For a semicoherent interface as in Cu/Ni boundaries, the well-aligned misfit dislocations may relax the coherency stresses at some distance away from the interface [2,10,12]. Under mechanical loading, these misfit dislocations can act as sources or preferred sites to nucleate lattice dislocations. For an incoherent interface such as the flat Kurdjumov-Sachs (KS) Cu{111}/Nb{110} (which we will refer to as "KS-F") and facetted KS Cu{112}/Nb{112} ("facetted KS{112}") interfaces [14,17–24], more complicated interfacial defect structures may provide more possible dislocation nucleation sites. The nucleation and emission of dislocations from such interfaces usually determine the dominant plasticity mechanism.

Recently, we demonstrated that it is possible to nucleate dislocations from the low energy, atomically flat KS-F interface [13,25–27], but a relatively high activation barrier must be overcome because all the intrinsic misfit dislocations have in-plane Burgers vectors [13,27]. In contrast, the equilibrium structure of the facetted KS{112} interface involves dissociated misfit dislocations extending into the Cu layers due to the existence of out-of-plane Burgers vectors [26,27], indicating a much lower barrier for dislocation nucleation. To account for the mechanical response to extreme loading conditions, large scale nonequilibrium molecular dynamics simulations were also carried out to investigate the effect of interface structure on the shock resistance [28]. This study found that the critical shock pressures to nucleate dislocations at such atomically flat KS-F interface are substantially higher than those from a facetted KS{112} interface, due to atomic-level interface characteristics that cause these two types of interfaces to nucleate, absorb and transmit dislocations by significantly different mechanisms. The flat KS-F interface provides a stress concentration in the

* Corresponding author.
E-mail address: zrf@buaa.edu.cn (R.F. Zhang).

http://dx.doi.org/10.1016/j.actamat.2016.05.015
1359-6454/

vicinity of the misfit dislocations that drives nucleation of a new Shockley partial loop [28], whereas the facetted KS{112} interface emits Shockley partial loops by direct dissociation of misfit dislocations. These findings suggest that Cu/Nb nanomultilayers with the flat KS-F interface are more shock resistant than those with the facetted KS{112} interface.

Under shear loading, interfacial sliding will play the dominant role, in addition to the aforementioned dislocation nucleation and emission processes. Through MD simulations, Wang et al. [29], Demkowicz et al. [30] and Zhou et al. [31] have separately demonstrated the stability of Cu-Nb interfaces subjected to shear deformations. It was shown that for the flat KS-F interface, simple shear leads only to interfacial sliding without emission of lattice dislocations, so these interfaces offer little shear resistance. For the facetted KS{112} interface, irrespective of shearing direction, plasticity consistently takes place inside the Cu layer and/or around the Cu-Nb heterointerfaces. The shear resistance of this interface is highly anisotropic, with interfacial sliding either occurring only at high stresses or not at all, and only dislocation emission observed [30]. These findings suggest a much higher shear resistance for the facetted KS{112} interface as compared to the flat KS interface, although the latter one possesses a higher activation barrier for dislocation nucleation.

In view of this trade-off of plastic resistance between "dislocation nucleation" and "interface sliding" for the flat KS-F and facetted KS{112} interfaces, one may ask whether it is possible to architect a heter/ogeneous interface that possesses both a high activation barrier for dislocation nucleation and a high resistance for interface sliding. In this work, we demonstrate that the introduction of appropriate atomic steps at the flat KS-F interface (transforming it into a stepped KS-S interface) may indeed achieve this goal. Such stepped KS-S interfaces are not merely theoretical possibilities, but have already been observed in as-synthesized Cu/Nb nanomultilayers. Fig. S1 in the Supplementary Material provides one example of an experimentally observed stepped KS-S interface with a single atomic step at the interface in accumulative roll bonding (ARB) samples [14,24], suggesting one possible fabrication route whose product can be subsequently optimized. Since this new type of interface possess two distinct characteristics: 1) a flat interface consisting of compact fcc{111}//{110}bcc planes, and 2) a discontinuity across this interface induced by an atomic step, we may expect such characteristics will cause the stepped KS-S interface to possess both a high activation barrier for dislocation nucleation and a high resistance for interface sliding.

To test this hypothesis, we investigate the dislocation nucleation and shear resistance of various stepped KS-S interfaces to understand how the steps influence the preferred nucleation sites and the slip system(s) they select, and the effect of steps on shear resistance. These are also compared with the widely studied flat KS-F and facetted KS{112} interfaces. Firstly, to understand the connection between interface structure and the subsequent nucleation mechanisms, we analyze the geometrical Schmid factor and interface defect factor to identify the most likely slip systems. The as-constructed stepped KS-S interfaces are then subjected to uniaxial tensile strain in three orthogonal directions to promote dislocation nucleation. We resolve several interesting issues concerning the preferred nucleation sites, and find that the stepped KS-S interface possesses a comparable (i.e., high) barrier for dislocation nucleation as compared to the flat KS interface. Secondly, the stepped KS-S interfaces are found to possess substantially more resistance to interface sliding, in a similar manner to the facetted KS{112} interface. The accommodation mechanism that propagates from the interface during shearing is found to be connected to the dissociation of the nucleated partial dislocations from interfaces, facilitating the formation and growth of the parallel twins or interface sliding under high stress, both of which dominate the deformation under shear loading.

2. Methodology and analytical technique

2.1. Interatomic potentials and simulation analysis

Empirical interatomic potentials for Cu and Nb and the interaction between Cu and Nb were constructed in the embedded atom method (EAM) framework [32]. In particular, we adopt the EAM potential developed by Voter and Chen [33] for Cu, and the Nb potential developed by Johnson and Oh [34]. These potentials have produced good results for surface diffusion and defect formation energies [35–37]. Since no significant ionic or directional covalent bonding is present between Cu and Nb, the interaction potentials designed to model bonding between these two elements are based on the usual form used for other metal pairs [38]. The fitting of such cross-potentials typically utilizes the dilute enthalpies of mixing [39] and/or the experimentally determined properties of intermetallic phases formed by these elements [33]. However, since the immiscible Cu-Nb system does not possess any intermetallic phases, the Cu-Nb cross potentials were instead constructed by Demkowicz et al. [40] by fitting the dilute enthalpies of mixing obtained from analytical fitting of the Cu-Nb phase diagram [41], as well as the lattice constant and bulk modulus of a hypothetical Cu-Nb crystal in the CsCl structure obtained by first principles calculations using the Vienna Ab-initio Simulation Package (VASP) [42].

Molecular dynamics simulations were performed with the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) code [43]. The common neighbor analysis and the atomic elastic strain is used to qualitatively visualize the dislocation structure inside the crystals, while the disregistry analysis are used to quantitatively analyze the dislocation core structure of an interface [10,27,32]. OVITO [44] and Atomeye [45] are used to visualize the atomic structure.

2.2. Models of bicrystal interfaces

Atomistic simulations are carried out to first establish the structures of the relaxed equilibrium Cu-Nb KS interface. A bicrystal model is created and assembled from two unrelaxed semi-infinite perfect crystals with the KS orientation relation, as shown in Fig. 1a. According to the KS orientation relationship the bilayer model has $(111)_{Cu}//(110)_{Nb}$ and $[11\text{-}2]_{Cu}//[1\text{-}12]_{Nb}$ and $[1\text{-}10]_{Cu}//[\text{-}111]_{Nb}$. The x-axis is along $[11\text{-}2]_{Cu}$, the y-axis is along $[111]_{Cu}$ and the z-axis is along $[1\text{-}10]_{Cu}$. The interface plane is the x-z plane, and periodic boundary conditions are applied in both the x and z directions. Because of the incommensurate nature of the Cu and Nb crystals, these two transverse dimensions are chosen such that the strains imposed on the Cu and Nb semi-infinite perfect crystals are small, while ensuring the equilibrium of forces. In the case of bicrystal interfaces, such equilibrium implies that the normal stresses $\boldsymbol{\sigma_{yy}}$ in both crystals are zero, and the summation of the transverse stresses σ_{xx} and σ_{zz} in the two crystals are both zero.

Relaxation of the bicrystal model is accomplished by two procedures, namely rigid body translation of one crystal with respect to the other and a full relaxation of the stress and atomic forces. In rigid body translation, the two crystals are able to translate as rigid bodies, in three directions, but not rotate. The net forces, acting parallel and perpendicular to the interface, drive the translations. Afterwards, a relaxation of stress and atomic positions is performed until the aforementioned stress conditions are satisfied, and the maximum force acting on any atom does not exceed 2 pN.

To create a step along the crystallographic $<110>_{Cu}$ direction at the interface, two types of crystallographic planes {111} and {001}