Acta Materialia 143 (2018) 107–120

Contents lists available at ScienceDirect

Acta Materialia

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

Full length article

Effect of dynamic evolution of misfit dislocation pattern on dislocation nucleation and shear sliding at semi-coherent bimetal interfaces

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ARTICLE INFO

Article history:
Received 25 July 2017
Received in revised form
27 September 2017
Accepted 4 October 2017
Available online 5 October 2017

Keywords:
Dynamic evolution
Misfit dislocation pattern
Bimetal
Interfaces
Dislocation nucleation
Shear sliding

ABSTRACT

Misfit dislocation pattern is generally accepted to play a critical role on the interface mediated deformation mechanism such as dislocation nucleation and shear sliding in various flat interfaces, however, a specific mechanical loading may dynamically modify its distribution and character before the appearance of distinct plastic flow out of interfaces. Taking bimetal semi-coherent interfaces with high symmetrically distributed misfit dislocations as an illustration, we reveal for the first time that the dynamic evolution of misfit dislocation patterns in interface appears for some specific interface types and loading schemes, and eventually governs the preferred sites of dislocation nucleation and the shear sliding mechanism. In contrary to the nearly unchanged feature of misfit dislocations under biaxial in-plane tension, the initial patterns around nodes of misfit dislocations are found to be distorted and spread anisotropically within interface during uniaxial in-plane loading, which in turn governs the non-Schmid phenomena of dislocation nucleation. A similar dependence of shear sliding mechanism on the anisotropic feature of core spreading of misfit dislocations in interface is also observed, depending on the characteristic of misfit dislocation patterns. Further investigations suggest that the dynamic evolution of misfit dislocation patterns may differ substantially for different types of interfaces, and consequently contribute to different mechanisms of dislocation nucleation and shear sliding. These results suggest a necessity to investigate the dynamic evolution of misfit dislocation patterns to get a more realistic understanding on the interface dominated plasticity.

1. Introduction

Metallic nanocomposites exhibit a lot of extraordinary mechanical properties, including high strength and high plastic deformability, superior shock and radiation damage resistance, which is closely correlated to the nanoscale confinement and the appearance of various types of interfaces or grain boundaries [1–14]. As the length scale is reduced from microscale to nanoscale, interfaces become a major carrier for plasticity of nanosized materials because the interface will provide sources for dislocation nucleation and the plasticity channel via interface sliding [7,11,12]. In general, the mechanism of dislocation nucleation and interface sliding can be understood according to interface dislocation theory and the geometrical analysis based on Schmid factor [4,5,7,9,10,14–20]. However, an atomistic understanding of dislocation nucleation and interface sliding is far more complicated, which depends strongly not only on the interface structure and intrinsic properties of adjoining metals, but also on the loading schemes [21–23].

In the case of coherent interfaces, dislocation nucleation is known to be difficult since the nucleation must overcome a high-energy barrier associated with the destruction of interface coherency. In contrast, the dislocation nucleation at a semi-coherent or incoherent interface is much easier, since the misfit dislocations and interface disconnections can relax the coherency and act as sources for nucleation of lattice dislocations [7,12,13,24]. Using molecular dynamics (MD) simulations, several unique interfaces dominated deformation mechanisms have been recently explored

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https://doi.org/10.1016/j.actamat.2017.10.012
1359-6454/

for some interface systems, including the interface-dependent non-Schmid effect that is attributed to the character of misfit dislocation. Among the multiple slip systems with the largest Schmid factor, it was found that the specific slip system activated depends on the distribution and character of misfit dislocations at Cu-Nb incoherent interface [22,23]. Latter, Salehinia et al. observed a similar nucleation behavior at metal-ceramic Nb-NbC interfaces [25]. In order to account for such non-Schmid phenomena, a geometrical model was recently proposed based on key structural relationships between the interface and adjoining crystal, to predict the most likely nucleation site from a given interface [21,26]. This study underlines that only those slip systems whose slip traces are parallel to a misfit dislocation line are activated even though multiple slip systems are available according to Schmid factor analysis. When the misfit dislocation lines are not parallel to the traces of the slip planes in the interface, the lattice dislocations could nucleate along dislocation junctions lying parallel to one of the slip traces in the interface. These junctions are formed via a reaction between intersecting misfit dislocations under mechanical loading [26,27]. Although a correlation among dislocation nucleation, interface sliding and misfit dislocation patterns has been built up, one critical issue is still left that all these studies are based on the geometrical analysis of interface structure and the character of misfit dislocations at equilibrium, but the dynamic evolution of the misfit dislocations in interface is generally ignored. Note that the term “dynamic evolution” is concerned with the analysis of atomic force and movement in atomic simulations either via energetic minimization or simulation at finite temperature, which has effect on the evolution of misfit dislocation patterns under loadings and consequently governs the nucleation mechanism and interface shearing. As will be clarified in the present paper, a distinct modification of misfit dislocation patterns in the interface may substantially change the nucleation mechanism, providing an in-depth understanding on the unexpected non-Schmid phenomena, and therefore it is necessary to investigate the dynamic evolution of misfit dislocation patterns and its determination on the dislocation nucleation and interface sliding.

In the case of the flat interfaces such as fcc{111}//{110}bcc and fcc{111}//{111}fcc, the interface plane corresponds to one glide plane of the constitute metal, and consequently the misfit dislocations have an extended core in the interface [24,28]. Under mechanical loading, the core structure and line sense of misfit dislocation may easily change by expansion/contraction, dissociation or recombination in the interface, which will depend strongly on the type of external loading. For instance, Shao et al. [28,29] have recently pointed out that there are four misfit dislocation patterns at Cu-Ni interfaces under the condition of full relaxation and biaxial in-plane tension/compression. They found that various unique node structures of misfit dislocations may appear and have a profound effect on the behavior of dislocation nucleation. However, such analysis is based on the assumption that distinct dynamic evolution of misfit dislocations does not exist during biaxial in-plane tensions/compression. As will be shown in the present studies, such precondition does not always apply for cases such as uniaxial stress, nonsymmetrical loadings and different types of interfaces. In addition, with further consideration of the intrinsic parameters of adjoining metals such as the misfit state and stacking fault energy difference, one would wonder if these factors will substantially contribute to the modification of the misfit dislocation patterns and its dominated dislocation nucleation or shear sliding in such interfaces, e.g. the representative fcc{111}//{111}fcc semi-coherent interface. The choice of fcc{111}//{111}fcc semi-coherent interface is based on the following three considerations: (i) a highly symmetrical distribution of misfit dislocations with the same character allows a comparative investigation on the choice of preferred slip system; (ii) different combinations of bimetal systems with distinct characteristics of interface structure, e.g. Cu-Ni, Cu-Ag and Ag-Pd, are available for systematic analysis; (iii) the interface sliding with suppression of dislocation nucleation may be easily implemented via shear loading, which provides a possibility to compare the shear sliding mechanism of this interface with that of the well-studied fcc{111}//{110}bcc incoherent interface.

In this work, we first investigate the misfit dislocation patterns at three representative fcc{111}//{111}fcc interface systems. The formation of different misfit dislocation patterns will be analyzed based on the misfit state and stacking fault energy difference of the bimetal interfaces. Secondly the dislocation nucleation under different loading schemes is demonstrated by means of atomistic simulations, in order to explore the correlation between the dislocation nucleation and the misfit dislocation patterns at equilibrium. To underline the unexpected or abnormal phenomena of dislocation nucleation, the dynamic evolution of misfit dislocation patterns will be further explored in order to demonstrate its controllable effect on the dislocation nucleation and a novel mechanism of dislocation nucleation in the interface is presented. Afterwards, we reveal that the dynamic evolution of misfit dislocation patterns also dominates the sliding mechanism of interface by the localized modification of core structure of misfit dislocation according to different paths of dissociation and recombination within the interface, which shows big difference for the different type of interfaces. A final discussion and remark is provided according to a detailed comparison with another widely studied fcc {111}//{110}bcc interface.

2. Methodology

2.1. Interface models

The fcc{111}//{111}fcc bi-layer models employ the same coordinate system for the two adjoining crystals, i.e. the x-axis along $[11\bar{2}]$, the y-axis along [111], and the z-axis along $[1\bar{1}0]$. The x-z plane is chosen as the interface plane. Periodic boundary conditions are imposed on both the x and z directions, while the semi-rigid boundary condition is applied for the y direction, in order to minimize the internal stress of the interfaces [11]. The dimensions of the simulation models are chosen to be 17.2 nm, 24.0 nm, 10.0 nm for Cu-Ni bilayer and 10.0 nm, 24.0 nm 5.8 nm for Ag-Pd bilayer, and 15.6 nm, 24.0 nm, 9.0 nm for Cu-Ag bilayer in the x, y, z directions respectively.

In Fig. 1, the unrelaxed Cu{111}//{111}Ni interface is illustrated, followed with an opened Thompson tetrahedron which will be used in our latter analysis of possible slip systems. Because of the misfit state between the two crystals depending on the different lattice constants, the unrelaxed Cu{111}//{111}Ni interface presents various distinct characteristics of local atomic structure. Four types of localized atomic structure are presented in Fig. 1a and characterized as: near-FCC region ($A_{Cu}B_{Cu}C_{Ni}A_{Ni}$), near-HCP region ($A_{Cu}B_{Cu}A_{Ni}B_{Ni}$), HESF region (high-energy stacking fault structure between the 1st Ni and 1st Cu layers, $A_{Cu}B_{Cu}B_{Ni}C_{Ni}$), and the highly distorted regions that separate the former three regions [30]. The formation of such kind of interface arrangement can be attributed to the introduction of Shockley partial dislocations into a coherent interface with coincidence site lattice (CSL) at the fcc{111}//{111}fcc interfaces (Fig. 1a and b). A geometrical analysis has been performed to characterize the distribution and Burgers vectors of the misfit dislocations in interface based on the combination of O-lattice theory proposed by Bollmann [31] and atomically informed Frank-Bilby theory (AIFB) proposed by Wang et al. [32]. It should be noted that recent works [33–35] indicated that the partitioning of