Computational Materials Science 44 (2008) 721–727

Contents lists available at ScienceDirect

Computational Materials Science

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

# Theoretical study of misfit dislocation in interface dynamics

Y. Long [a,b,*], N.X. Chen [a,c]

[a] Department of Physics, Tsinghua University, Beijing 100084, China
[b] Center for Advanced Study, Tsinghua University, Beijing 100084, China
[c] Institute for Applied Physics, University of Science and Technology, Beijing 100083, China

ARTICLE INFO

*Article history:*
Received 21 February 2008
Received in revised form 2 May 2008
Accepted 19 May 2008
Available online 9 July 2008

*PACS:*
61.72.Lk
68.35.Ja

*Keywords:*
Misfit dislocation
Interface dynamics
Dislocation velocity

ABSTRACT

Misfit dislocation is an important component of the semi-coherent interface. It is a line defect on interface, and strongly affects the structural and dynamical properties. In this work, we use an atomistic simulation method to study two representative dynamics of Pd/MgO interface: the fracture and slipping. The calculation shows that for both the two cases, misfit dislocation plays a critical role. However, the dislocation in the latter is much more important than in former, that it reduces the tensile stress (in fracture) for 26% but slip stress (in slipping) for three orders of magnitude. Also, some valuable parameters of misfit dislocation can be extracted from the atomistic simulation results by a simple derivation, such as the dislocation width, mass and velocity, which are determined as 14 Å, 0.46 awu/Å and 40 m/s in this work.

## 1. Introduction and methodology

Metal/oxide interface is an important issue in current materials science and technology. It has special physical and chemical properties on the interface plane, and plays a crucial role in many technical applications such as catalysts, composites and metal–ceramic sensors etc [1–4], so asks for theoretical studies. However, the conventional first principle method is usually limited in ideal interface models, but is less applicable in some complex problems such as misfit dislocation and wetting. At this condition, people call for atomistic study based on model potentials.

In this work, we use an atomistic simulation method to study the fracture and slipping processes of Pd/MgO(001) interface, mainly pay attention to the function of misfit dislocation. As we known, dislocation is the key point of plastic deformation for bulk metals, but how it works on interface between metal and oxide? Especially, misfit dislocation in a semi-coherent interface is more dense than it in bulk materials, and usually arranged in a regular dislocation network. So it also may play an important role in interface dynamics, and this is our purpose in atomistic study.

About the Pd/MgO(001) interface considered in this work, it is a fcc/rocksalt structure, with the lattice constant $a_{\mathrm{Pd}} = 3.89$ Å for Pd and $a_{\mathrm{MgO}} = 4.22$ Å for MgO [5], so the misfit is $2\frac{a_{\mathrm{MgO}}-a_{\mathrm{Pd}}}{a_{\mathrm{MgO}}+a_{\mathrm{Pd}}} = 8.1\%$. However, we choose Pd/MgO as the target system because it is a widely studied topic both in experiments and theoretics [6–13], and the Burgers vector ($b$) for misfit dislocation is experimentally determined as $\frac{a_{\mathrm{Pd}}}{2}[1\,1\,0]$ [14–17]. Also, in our previous works [18,19], we have gotten some basic structural properties of misfit dislocation in Pd/MgO(001). The dislocation line (DL) is determined as in the first monolayer (ML) of metal side, with metal atoms on hollow side for dislocation core area, and on *O* site for interface coherent area, as shown in Fig. 1. Based on these results, we can proceed the advanced study easily.

For the atomistic study in this work, we consider a two dimensional cross-section model for Pd/MgO(001) interface, just as we have done before [18]. Usually, the fracture or slipping of a certain interface takes place at the interface plane, so it is weakly associated with the MLs far away from this plane. For convenience, we take six MgO MLs and 10 Pd MLs for the interface model in calculation. This is because DL is placed on interface, 10 MLs in Pd side is enough to support the misfit dislocation, and MgO as an ionic crystal, six MLs is enough.

In order to study the fracture and slipping processes atomistically, we divide them into a series of medium steps, and use an energy minimization program [20] to study each step. In this method, the last MLs of Pd and MgO are fixed in energy minimization. And in each step, the final ML in Pd side is vertically (for fracture) or parallel (for slipping) moved for a small distance, while the other atoms are relaxed under the interatomic potentials. At this condition, we use $x$ as the tensile distance and $y$ as the slip distance, as

---

* Corresponding author. Address: Department of Physics, Tsinghua University, Beijing 100084, China. Fax: +86 010 62772783.
*E-mail address:* longyao@tsinghua.org.cn (Y. Long).

doi:10.1016/j.commatsci.2008.05.022

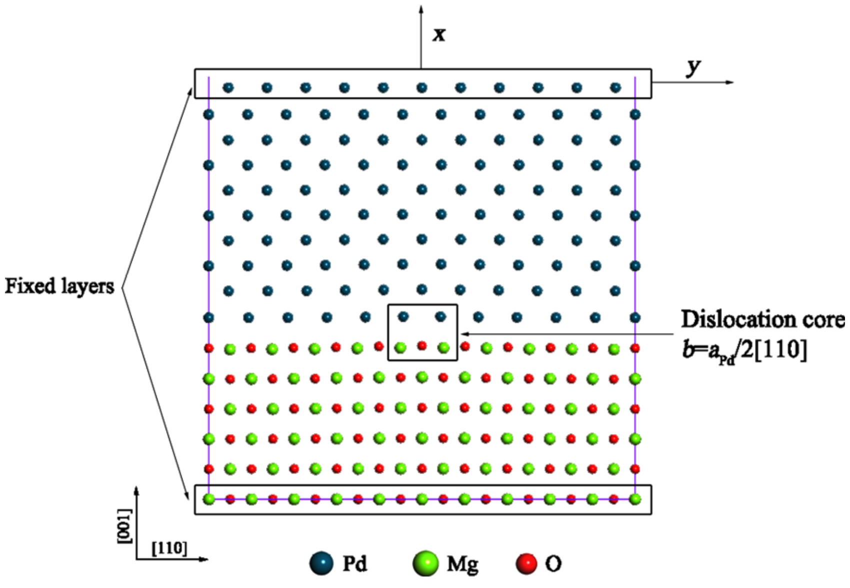

**Fig. 1.** The cross-section model of Pd/MgO(001) interface, where misfit dislocation is placed in the first ML of metal side.

shown in Fig. 1. For *x* or *y* increases from zero to several angstroms, we can draw a picture of the interface fracture or slipping process.

The following work consists of three parts. First, in Section 2, we introduce the interatomic potentials used in this work. They are pair potentials obtained by a Chen–Möbius inversion method, including both the terms across interface and inner bulk materials. Although this is a very simple pair potential approach, we show that it is quite practical for the interface system and sometimes reasonable. Next, in Section 3, we proceed atomistic studies to the interface dynamics mentioned above. This is the main part of the present work. We start from the atomistic simulation of a representative model, go deep into some general rules of the interface fracture and slipping processes, and result in an evaluation of the dislocation width, mass and velocity. At last, Section 4 is the conclusion.

## 2. Interatomic potentials

Interatomic potential is the first important issue in atomistic simulation. It gives an energetic description of the target system in a certain approximation, and so can proceed some conventional atomistic studies such as energy minimization or molecular dynamics. However, its validity directly determines the credibility of simulation result, and its simplicity relates to the calculation effort. So a practical and reasonable potential model is desired for interface systems.

In this work, we use a pair potential approach to study the Pd/MgO interface. These are ab initio based pair potentials obtained by a Chen–Möbius inversion method [18,21–23], extracted from ab initio cohesive or adhesive energies by a certain inversion formula. More accurately, we use the cohesive energy curves in uniform expansion to get the metal–metal and oxide–oxide potentials for Pd and MgO lattices, and use the adhesive energy curves in tensile test to get the metal–oxide potentials for Pd/MgO interface. In this method, the pairwise assumption is widely used. It seems a very simple approximation for the metal/oxide interface, but is quite practical and can give a reasonable description of the problems we are interesting in, as checked in the following part.

The Pd/MgO interface contains three kinds of interatomic potentials: the metal–oxide terms $\Phi_{\mathrm{Pd-O}}$ and $\Phi_{\mathrm{Pd-Mg}}$, metal–metal term $\Phi_{\mathrm{Pd-Pd}}$, and oxide–oxide terms $\Phi_{\mathrm{O-O}}$, $\Phi_{\mathrm{Mg-Mg}}$ and $\Phi_{\mathrm{Mg-O}}$. For an intuitive view, Fig. 2 shows their potential curves. Note that the curves for oxide–oxide interactions are quite different from the others. This is because these potentials for ionic crystal contain both the short-range and long-range parts (that the latter is coulomb interaction), while the metal–metal and metal–oxide ones are just short-range potentials. Further more, about the metal–oxide interactions across interface, $\Phi_{\mathrm{Pd-O}}$ is attractive, and $\Phi_{\mathrm{Pd-Mg}}$ is repulsive. This relation is useful for the latter discussion, so mentioned beforehand. At last, about the potential parameters, the metal–oxide and oxide–oxide ones are just following the previous works [18,23], but the metal–metal one is recalculated from ab initio level for an improvement, resulted in a Rahman–Stillinger–Lemberg potential (Eq. (1)), as shown in Table 1.

$$\Phi = D_0 e^{y\left(1-\frac{r}{R_0}\right)} + \frac{a_1}{1+e^{b_1(r-c_1)}} + \frac{a_2}{1+e^{b_2(r-c_2)}} + \frac{a_3}{1+e^{b_3(r-c_3)}}. \qquad (1)$$

In order to understand the validity of the above potentials, we check the metal–metal and metal–oxide ones on some basic elastic and energetic properties, such as the lattice constant ($a$), elastic constants ($C_{11}$, $C_{12}$ and $C_{44}$), cohesive energy ($\varepsilon$) and surface energy ($\gamma$), as shown in Table 2. For this checking, the theoretical values

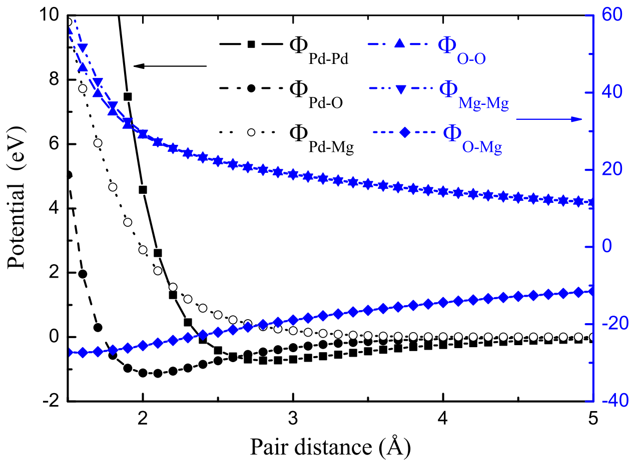

**Fig. 2.** Potential curves of $\Phi_{\mathrm{Pd-Pd}}$, $\Phi_{\mathrm{O-O}}$, $\Phi_{\mathrm{Mg-Mg}}$, $\Phi_{\mathrm{O-Mg}}$, $\Phi_{\mathrm{Pd-O}}$ and $\Phi_{\mathrm{Pd-Mg}}$.