Pair potential approach for metal/Al_2O_3 interface

2007 J. Phys.: Condens. Matter 19 196216

(http://iopscience.iop.org/0953-8984/19/19/196216)

IOP PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **19** (2007) 196216 (11pp) doi:10.1088/0953-8984/19/19/196216

Pair potential approach for metal/Al_2O_3 interface

Y Long[1] **and N X Chen**[1,2]

[1] Department of Physics, Tsinghua University, Beijing 100084, People's Republic of China
[2] Institute for Applied Physics, University of Science and Technology, Beijing 100083, People's Republic of China

E-mail: longyao@tsinghua.org.cn

Received 5 March 2007, in final form 22 March 2007
Published 19 April 2007
Online at stacks.iop.org/JPhysCM/19/196216

Abstract

The atomistic simulation of a metal/oxide interface is a challenge in surface science and technology. It requires a systematic way of obtaining the interatomic potentials across the interface. In this work, we use a Chen–Möbius inversion method to study the Ni/Al_2O_3 interface, and get a concise and general inversion formula, which is used to extract pair potentials from *ab initio* adhesive energies. A series of checks show that the inversed potentials are self-consistent and also partially transferable. These potentials prefer to treat the Al terminated interface, but are not so good for the O terminated interface. In summary, the present work provides a novel way to get the *ab initio* based pair potentials across an interface, with the derivation of an inversion formula of both theoretical and practical importance.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Nowadays, metal/oxide interfaces play an important role in catalysts, electronic packaging and high-temperature structural ceramics etc. Among them, metal/Al_2O_3 interface is a widely used and studied case. However, its complex interfacial structure makes the theoretical study of it very difficult. It is a challenge to get a reasonable atomistic description of a metal/Al_2O_3 interface.

Factually, there have been many theoretical studies on metal/Al_2O_3 interfaces, by the use of *ab initio* calculations and molecular dynamics simulation respectively. The former concentrates on the basic interfacial properties such as interfacial distance, metastable structure and adhesion work etc [1–6], while the latter can work on some complex problems such as the interfacial misfit dislocation [7–10]. Considering the advantages and shortcomings of previous works, we use a Chen–Möbius inversion method to work on this topic.

In this work, we obtain a concise inversion formula for a Ni/Al_2O_3 interface, and then use it to extract the free-standing interfacial potentials from *ab initio* adhesive energies. This is a

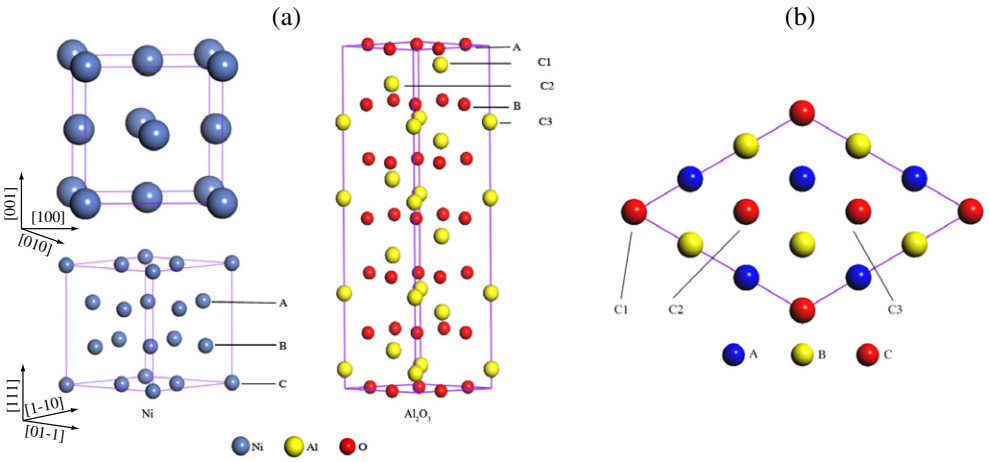

Figure 1. (a) The lattice structures of Ni and Al_2O_3. (b) The three ML types A, B and C in Ni and Al_2O_3 lattices.

part of the systematic work in the frame of the Chen–Möbius inversion method, which began in the 1990s with Chen [11] and has gone through ionic crystals [12], rare earth compounds [13], semiconductors [14] and metal/MgO interfaces [15, 16].

This paper consists of three parts. First, section 2 shows the derivation of an inversion formula for a Ni/Al_2O_3 interface. This is the main purpose of the present work and the resultant formula is of both theoretical and practical importance. Next, in section 3, by using the pre-determined inversion formula, we extract the interfacial potentials from *ab initio* adhesive energies. A comprehensive countercheck shows that the inversed potentials are self-consistent and partially transferable. Finally, section 4 is the conclusion.

2. Methodology

The Chen–Möbius inversion method is a pair potential approach to the target system, including bulk and interface, in which the total cohesive or adhesive energy is assumed equal to the summation of all pair interactions. This pair potential model looks like a simple approximation, but it is quite practical and usually gives a reasonable description of the complex system including metal/oxide interfaces [15, 16]. Now, we use this method to study a Ni/Al_2O_3 interface.

2.1. Lattice structures

Before deriving the inversion formula, the lattice structures of Ni and Al_2O_3 should first be introduced. As we known, Ni has a fcc lattice, with the lattice constant $a = 3.5239$ Å and Al_2O_3 has a hcp lattice, with $a = 4.7591$ Å and $c = 12.9894$ Å, see figure 1(a).

In a detailed description of the lattice structures, we classify the monolayers (MLs) of Ni and Al_2O_3 into several types. First, the MLs in the Ni lattice along the (111) direction are in an A–B–C arrangement, where A, B and C denote different kinds of MLs, as shown in figure 1(b). Second, the MLs in the Al_2O_3 lattice are sometimes more complex than in Ni. Along the (0001) direction, O MLs and Al MLs appear alternately, and there are two Al MLs following one O ML, see figure 1(a). The O MLs are in an A–B arrangement and the Al MLs are in a

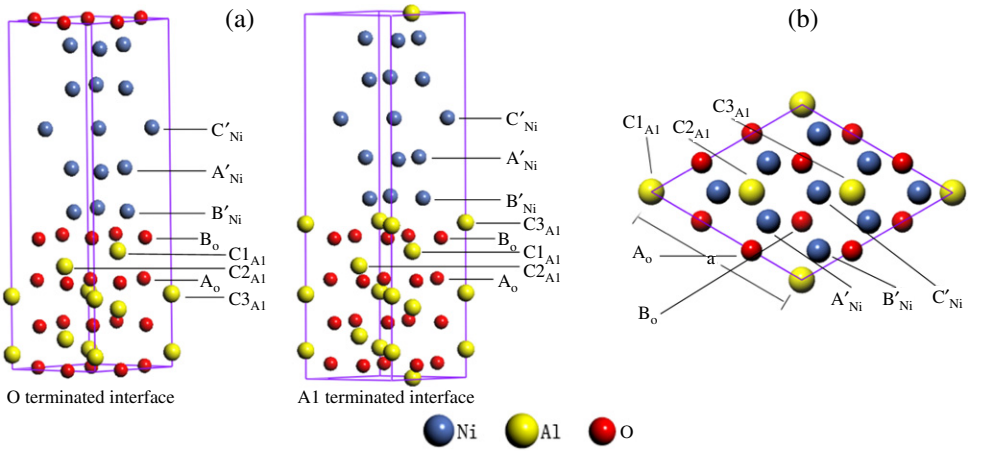

Figure 2. The specially designed Ni/Al_2O_3 interfacial structures. (a) The O terminated and Al terminated interfaces. (b) Interfacial structures in the [0001] direction. Note that the MLs of Ni side are denoted as A′, B′ and C′ in these interfacial models.

C1–C2–C3 arrangement, where C1, C2 and C3 denote one third part of C-type ML, as shown in figure 1(b). This is because the atom number in Al ML is one third of that in C-type ML.

For some more information, the vertical distances between the nearest MLs in Ni and Al_2O_3 lattices can be derived from the lattice constants, which are $d_1 = 2.035$ Å for Ni and $d_2 = 0.7216$ Å for Al_2O_3. They are used in deriving the inversion formula. Furthermore, the misfit of the Ni/Al_2O_3 interface is 9.3%, which is obtained by the formula:

$$\frac{a_{Al_2O_3} - \sqrt{\frac{3}{2}}a_{Ni}}{a_{Al_2O_3}}. \tag{1}$$

Note that our inversion formula is built on the ideal interfacial models. So the Ni lattice is extended to fit the Al_2O_3 lattice, Al_2O_3 is an ionic crystal which is much more rigid than metal.

2.2. Inversion formula

There are two kinds of pair potentials Φ_{Ni-O} and Φ_{Ni-Al} across the interface, so we need two interfacial models to derive the inversion formula, with O terminated and Al terminated of the Al_2O_3 side respectively (or briefly, O terminated and Al terminated interfaces), see figure 2(a). Factually, these interfacial structures are specially designed in the requirement of deriving a concise inversion formula, as shown in figure 2(b). The Ni atom is not just on top of O or Al sites, but it has been moved away from the O site for $\frac{a}{9}$ along the [1000] direction and $-\frac{a}{9}$ along the [0100] direction, where $a = 4.7591$ Å is the lattice constant of Al_2O_3. In particular, the MLs of the Ni side are denoted as A′, B′ and C′, to be distinguished from the ones before moving.

Now, we study the ML-interactions of the two interfacial models, which are equal to the summation of all the pair interactions between two MLs across the interface. For the Ni/Al_2O_3 interface, there are three kinds of Ni MLs (A'_{Ni}, B'_{Ni} and C'_{Ni}), two kinds of O MLs (A_O and B_O) and three kinds of Al MLs ($C1_{Al}$, $C2_{Al}$ and $C3_{Al}$), resulting in 15 kinds of ML interactions ($3 \times (2 + 3)$): A'_{Ni}–A_O, A'_{Ni}–B_O, A'_{Ni}–$C1_{Al}$, A'_{Ni}–$C2_{Al}$, A'_{Ni}–$C3_{Al}$, B'_{Ni}–A_O, B'_{Ni}–B_O, B'_{Ni}–$C1_{Al}$, B'_{Ni}–$C2_{Al}$, B'_{Ni}–$C3_{Al}$, C'_{Ni}–A_O, C'_{Ni}–B_O, C'_{Ni}–$C1_{Al}$, C'_{Ni}–$C2_{Al}$ and C'_{Ni}–$C3_{Al}$. However, the energy expressions of these fifteen ML interactions have a simple form, for all

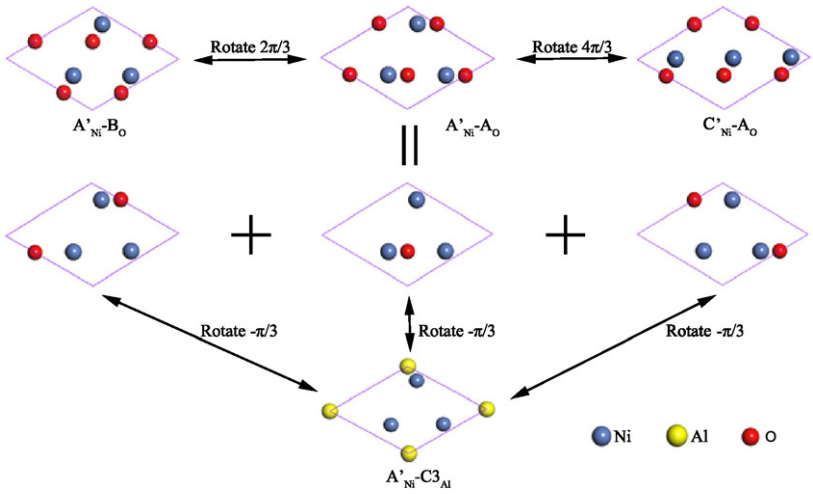

Figure 3. The geometrically identical relationships between some ML pairs, in the [0001] direction. Note that the ML pairs are two-dimensional periodic structures, here we just present a unit cell.

the Ni–O ML-pairs (or Ni–Al) are geometrically identical through a rotation or translation. This is a critical relationship brought by the designation of interfacial structures, from which we can derive a concise inversion formula easily.

Figure 3 shows this identical relationships between $A'_{Ni}-B_O$, $A'_{Ni}-A_O$ and $C'_{Ni}-A_O$ ML pairs as the examples. Also, it demonstrates that $A'_{Ni}-A_O$ ML pair can be divided into three parts, with each part identical to $A'_{Ni}-C3_{Al}$ ML pair through a rotation of a certain angle. Based on these examples, we give a comprehensive description of the geometric identical relationships: all the Ni–O (or Ni–Al) ML pairs are identical through a rotation or translation, and each Ni–O ML pair can be divided into three parts with each part identical to a Ni–Al ML pair.

From the above discussion, we can use a common expression to describe the Ni–O and Ni–Al ML interactions:

$$H_{\mathrm{Ni-O,Ni-Al}}(x) = \sum_{m,n=-\infty}^{\infty} \Phi_{\mathrm{Ni-O,Ni-Al}}\left(\sqrt{x^2 + \frac{a^2}{3}\left(m^2 + \left(n-\frac{1}{3}\right)^2 + m\left(n-\frac{1}{3}\right)\right)}\right) \quad (2)$$

where x denotes the vertical distance between MLs, m and n refer to the atomic indices parallel to the interfacial plane. As the atom number of O ML is three times that of Al ML, the Ni–O ML-interaction is $3H_{\mathrm{Ni-O}}(x)$, while it is $H_{\mathrm{Ni-Al}}(x)$ for Ni–Al ML pairs. By the way, equation (2) is our achievement in the designation of interfacial structures. It provides us with a concise formula of the Ni–O and Ni–Al ML-interactions.

By using the ML interactions $H_{\mathrm{Ni-O}}(x)$ and $H_{\mathrm{Ni-Al}}(x)$, we get a concise expression of adhesive energies, with the corresponding interfacial structures presented in figure 2:

$$\begin{aligned} E_{\mathrm{O}}(x) = &\sum_{m=0,n=0}^{\infty} (3H_{\mathrm{Ni-O}}(x + md_1 + 3nd_2) + H_{\mathrm{Ni-Al}}(x + md_1 + (3n+1)d_2) \\ &+ H_{\mathrm{Ni-Al}}(x + md_1 + (3n+2)d_2)) \\ E_{\mathrm{Al}}(x) = &\sum_{m=0,n=0}^{\infty} (3H_{\mathrm{Ni-O}}(x + md_1 + (3n+1)d_2) + H_{\mathrm{Ni-Al}}(x + md_1 + 3nd_2) \\ &+ H_{\mathrm{Ni-Al}}(x + md_1 + (3n+2)d_2)) \end{aligned} \quad (3)$$

where E_O and E_{Al} denote the adhesive energies of O terminated and Al terminated interfaces respectively, m and n refer to the ordinal numbers of MLs in the Ni and Al_2O_3 sides and x denotes the interfacial distance—which is the vertical distance between two nearest MLs across the interface.

For simplifying the energy expressions, we define three vectors:

$$E(x) = \begin{bmatrix} E_O(x) \\ E_{Al}(x) \end{bmatrix}, \qquad H(x) = \begin{bmatrix} H_{Ni-O}(x) \\ H_{Ni-Al}(x) \end{bmatrix}, \qquad \Phi(x) = \begin{bmatrix} \Phi_{Ni-O}(x) \\ \Phi_{Ni-Al}(x) \end{bmatrix}. \tag{4}$$

As a result, equation (3) can be rewritten as:

$$E(x) = \sum_{m,n=0}^{\infty} A_{m,n} H(x + md_1 + nd_2) \tag{5}$$

where $A_{m,n}$ is a 2×2 matrix, for example, $A_{0,0} = \left[\begin{smallmatrix} 3 & 0 \\ 0 & 1 \end{smallmatrix}\right]$.

The solution of equation (5) is obtained by calculating the inversion coefficient $B_{m,n}$, which satisfies:

$$\sum_{m,n=0}^{M,N} B_{m,n} A_{M-m,N-n} = \delta_{M,0}\delta_{N,0}, \qquad \forall M, \quad N \in \overline{\mathbb{Z}^-}. \tag{6}$$

Based on equations (5) and (6), we can prove that:

$$\begin{aligned} \sum_{m,n=0}^{\infty} B_{m,n} E(x + md_1 + nd_2) &= \sum_{m,n=0}^{\infty} B_{m,n} \sum_{m',n'=0}^{\infty} A_{m',n'} H(x + (m+m')d_1 + (n+n')d_2) \\ &= \sum_{M,N=0}^{\infty} \sum_{\substack{m+m'=M \\ n+n'=N}} B_{m,n} A_{m',n'} H(x + (m+m')d_1 + (n+n')d_2) \\ &= \sum_{M,N=0}^{\infty} \sum_{m,n=0}^{M,N} B_{m,n} A_{M-m,N-n} H(x + Md_1 + Nd_2) \\ &= \sum_{M,N=0}^{\infty} \delta_{M,0}\delta_{N,0} H(x + Md_1 + Nd_2) \\ &= H(x). \end{aligned} \tag{7}$$

So the ML interactions $H(x)$ are extracted from the adhesive energy $E(x)$:

$$H(x) = \sum_{m,n=0}^{\infty} B_{m,n} E(x + md_1 + nd_2). \tag{8}$$

Now, we need to extract the interfacial pair potentials from ML interactions to achieve a final inversion formula. For this purpose, equation (2) is rewritten as:

$$H(x) = \sum_{m,n=-\infty}^{\infty} \Phi\left(\sqrt{\left(x^2 + \frac{a^2}{27}\right) + \frac{a^2}{27}(9m^2 + (3n-1)^2 + 3m(3n-1) - 1)}\right). \tag{9}$$

Note that the item on the right-hand side $9m^2 + (3n-1)^2 + 3m(3n-1) - 1$ is always greater than or equal to 0, that is it is equal to 0 if and only if $m = 0$ and $n = 0$.

For simplifying equation (9), we define:

$$H'\left(\sqrt{x^2 + \frac{a^2}{27}}\right) = H(x) \tag{10}$$

so that we get:

$$H'(x) = \sum_{m,n=-\infty}^{\infty} \Phi\left(\sqrt{x^2 + \frac{a^2}{27}(9m^2 + (3n-1)^2 + 3m(3n-1) - 1)}\right)$$
$$= \sum_{k=0}^{\infty} a_k \Phi\left(\sqrt{x^2 + k\frac{a^2}{27}}\right) \tag{11}$$

where a_k is equal to the number of solutions for:

$$k = 9m^2 + (3n-1)^2 + 3m(3n-1) - 1, \qquad m, \quad n \in \mathbb{Z}. \tag{12}$$

The same as equations (5), and (11) is solved by the use of inversion coefficient b_k, which satisfies:

$$\sum_{n=0}^{k} a_n b_{k-n} = \delta_{k,0}, \qquad \forall k \in \overline{\mathbb{Z}^-}. \tag{13}$$

It can be proven that:

$$\sum_{k=0}^{\infty} b_k H'\left(\sqrt{x^2 + k\frac{a^2}{27}}\right) = \sum_{k=0}^{\infty} b_k \sum_{k'=0}^{\infty} a_{k'} \Phi\left(\sqrt{x^2 + (k+k')\frac{a^2}{27}}\right)$$
$$= \sum_{n=0}^{\infty} \sum_{k+k'=n} a_{k'} b_k \Phi\left(\sqrt{x^2 + (k+k')\frac{a^2}{27}}\right)$$
$$= \sum_{n=0}^{\infty} \sum_{k=0}^{n} a_{n-k} b_k \Phi\left(\sqrt{x^2 + n\frac{a^2}{27}}\right)$$
$$= \sum_{n=0}^{\infty} \delta_{n,0} \Phi\left(\sqrt{x^2 + n\frac{a^2}{27}}\right)$$
$$= \Phi(x). \tag{14}$$

So the interfacial potentials are extracted from ML interactions:

$$\Phi(x) = \sum_{k=0}^{\infty} b_k H'\left(\sqrt{x^2 + k\frac{a^2}{27}}\right)$$
$$= \sum_{k=0}^{\infty} b_k H\left(\sqrt{x^2 + (k-1)\frac{a^2}{27}}\right). \tag{15}$$

Considering equations (8), (10) and (15), the final inversion formula of the Ni/Al_2O_3 interface is obtained by using the inversion coefficients $B_{m,n}$ and b_k:

$$\begin{bmatrix} \Phi_{Ni-O}(x) \\ \Phi_{Ni-Al}(x) \end{bmatrix} = \sum_{m,n,k=0}^{\infty} b_k B_{m,n} \begin{bmatrix} E_O\left(\sqrt{x^2 + (k-1)\frac{a^2}{27}} + md_1 + nd_2\right) \\ E_{Al}\left(\sqrt{x^2 + (k-1)\frac{a^2}{27}} + md_1 + nd_2\right) \end{bmatrix}. \tag{16}$$

This inversion formula is the main purpose of the present work. It helps to extract the interfacial potentials from adhesive energies directly based on their energy expressions. Now, for a comprehensive understanding of the advantages and shortcomings of this method, we compare it with other work on the model potentials for metal/oxide interfaces.

First, a famous potential model of the metal/oxide interface is the discrete classical model, it was proposed by Duffy [17, 18] and Finnis [19] in 1992. The image charge across the

interface is carefully considered in this method, so it is suitable to study the interfaces of a large charge transfer. However, for a complex procedure in deriving the interatomic potentials, this method is mainly used in the cases of a simple interfacial structure, for example, the metal/MgO interfaces [20, 21].

The second one is the iteration method proposed by Yao [22]. The interatomic potentials are derived from *ab initio* adhesive energies by iteration. Its advantage is that the potentials are obtained without any prerequisite of the functional forms. But the iterative computation is time-consuming, and the convergence of the iterative program is also a difficult problem.

The third one is the fitting method. The potentials across the interface are fitted from *ab initio* adhesive energies by some optimization method, see Endou [23], Vervisch [24] and Dmitriev's [7–10] work. This method is more practical than the above two, so it has been widely used in metal/MgO and metal/Al_2O_3 interfaces. However, it also has a shortcoming that the potential functional form must be determined before fitting.

Considering the experiences of the previous works, we use a Chen–Möbius inversion method to work on the metal/Al_2O_3 interface. This method provides a concise and general inversion formula for the fcc-metal/Al_2O_3 interface, which helps us to derive interfacial potentials from *ab initio* adhesive energies without any prerequisite of their functional forms. The existence of an inversion formula can greatly reduce the effort in theoretical derivation and iterative computation. It is of both theoretical and practical importance. Also, this method has its limitation. For deriving the inversion formula, the interfacial models are specially designed, in which a metal atom is in a special site on the $Al_2O_3(0001)$ plane, see figure 2. Considering this fact, we need a comprehensive countercheck for the inversed potentials, as shown in the next section.

3. Results

Now, we are in a position to get the pair potentials across the Ni/Al_2O_3 interface by using the pre-determined inversion formula. For this purpose, the *ab initio* calculation is performed with the generalized gradient approximation (GGA) by using the CASTEP code [25, 26]. In parameter setting, the plane-wave cut-off energy is 340 eV and the k-point spacing is 0.05 Å^{-1}, generated by the Monkhorst–Pack scheme [27, 28].

Figure 4(a) shows the resultant potential curves of $\Phi_{\text{Ni-O}}$ and $\Phi_{\text{Ni-Al}}$. From the figure, we see that the Ni–O interaction is attractive and the Ni–Al interaction is repulsive. Then, these potentials are fitted into a Rahman–Stillinger–Lemberg (RSL2) functional form (equation (17)), with the related parameters listed in table 1.

$$\Phi = D_0 \mathrm{e}^{y(1-\frac{r}{R_0})} + \frac{a_1}{1+\mathrm{e}^{b_1(r-c_1)}} + \frac{a_2}{1+\mathrm{e}^{b_2(r-c_2)}} + \frac{a_3}{1+\mathrm{e}^{b_3(r-c_3)}}. \tag{17}$$

As the potentials have been obtained, a countercheck needs to be performed to show the credibility and reliability of these inversed potentials. For this purpose, we recalculate the original adhesive energies and search through some more interfacial models.

First, the original adhesive energies are recalculated by summing the pair interactions across the interface one by one and then compare them with the *ab initio* results, as shown in figure 4(b). From the figure, we see that the original *ab initio* adhesive energies are precisely reproduced by the inversed potentials through the total energy curves. This is the main purpose of the present work. It shows that the inversed potentials are self-consistent.

Next, for an advanced checking, we calculate the adhesive energies for a series of interfacial models by pair potentials and *ab initio* calculation comparatively. Here we consider six interfacial models, of Ni on an Al site, O site and hollow site (H site) respectively, for both

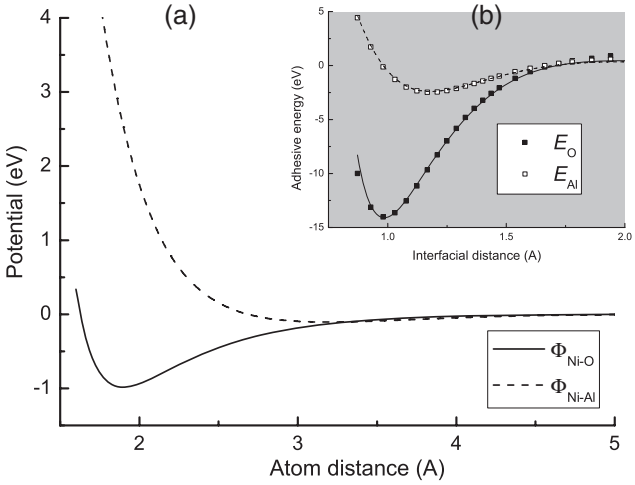

Figure 4. (a) Potential curves of Φ_{Ni-O} and Φ_{Ni-Al}. (b) Recalculating the original *ab initio* adhesive energies by the inversed potentials. The squares indicate the *ab initio* results, and the lines indicate the sum of pair potentials.

Table 1. Potential parameters of Φ_{Ni-O} and Φ_{Ni-Al}.

	Φ_{Ni-O}	Φ_{Ni-Al}
D_0 (eV)	171.67	55.70
R_0 (Å)	1.00	1.00
y	2.81	2.04
a_1 (eV)	−121.20	−7.76
b_1 (Å^{-1})	3.56	2.46
c_1 (Å)	1.19	1.65
a_2 (eV)	−15.91	−26.65
b_2 (Å^{-1})	2.37	1.48
c_2 (Å)	1.64	0.67
a_3 (eV)	0.01	0.05
b_3 (Å^{-1})	0.36	1.74
c_3 (Å)	0.33	4.97

the Al terminated and O terminated interfaces, as shown in figures 5 and 6. Note that these six models are different from the ones used for deriving the inversion formula (see figure 2). This calculation can check the transferability of the inversed potentials.

Figure 7 demonstrates the resultant adhesive energy against interfacial distance curves of Al terminated interfacial models as the examples. It shows that the adhesive energy curves obtained by the two ways are in good agreement for the Al site and O site models of the Al terminated interface. However, it is not so good for the other models, including the H site case and the O terminated interfacial models. This advanced checking shows a partial transferability of the inversed potentials. They cannot precisely reproduce the *ab initio* adhesive energies for all the representative structures of the Ni/Al_2O_3 interface, but can treat several cases.

In addition, we calculate the adhesion work (W_{ad}) for these interfacial models, which is extracted from the adhesive energy curve by using the formula:

$$W_{ad} = -\frac{\min\{E_{ad}\}}{S} \tag{18}$$

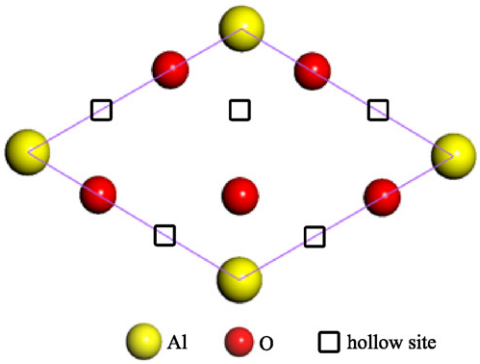

Figure 5. Three kinds of Ni sites for the Ni/Al_2O_3 interface: the O site, Al site and hollow site (H site). Here we just present the first O ML and Al ML.

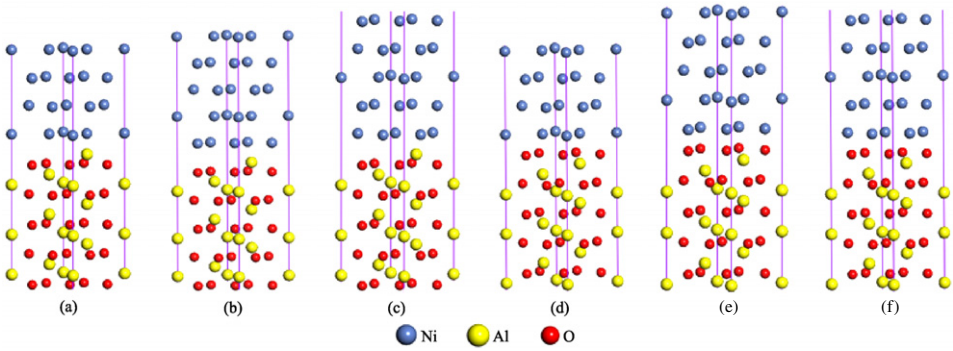

Figure 6. Six interfacial models for advanced checking. (a) Al terminated interface, Ni on Al site, (b) Al terminated interface, Ni on O site, (c) Al terminated interface, Ni on H site, (d) O terminated interface, Ni on Al site, (e) O terminated interface, Ni on O site, (f) O terminated interface, Ni on H site.

Table 2. W_{ad} for some interfacial models, obtained by inversed potentials and *ab initio* calculation respectively (J m^2).

	Al terminated			O terminated		
	Al site	O site	H site	Al site	O site	H site
By potentials	0.94	1.84	1.67	7.77	4.82	9.42
By *ab initio*	1.01	1.90	1.24	6.04	6.29	6.16

where $\min\{E_{ad}\}$ denotes the minimum value in the adhesive energy curve, and S denotes the interfacial area. Table 2 shows the resultant W_{ad} obtained by pair potentials and *ab initio* calculation. From the figure, we see that W_{ad} obtained by the two methods are in good agreement for the Al site and O site models of the Al terminated interface. However, it is not so good for the other cases, with a difference between 22% and 35%.

In summary, the inversed potentials are self-consistent and also have a partial transferability. They prefer to treat the Al terminated interface, because they can precisely reproduce the *ab initio* adhesive energies for two Al terminated interfacial models. However, they are not so good for the O terminated interface. This is the limitation of our method.

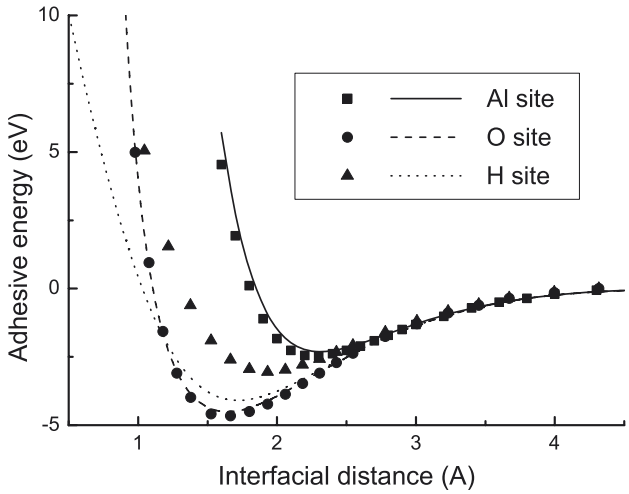

Figure 7. The adhesive energies obtained by inversed potentials and *ab initio* calculation for Al terminated interfacial models. The lines indicate the results from pair potentials and the scatter symbols indicate the ones from *ab initio* calculation.

4. Conclusion

In this work, a Chen–Möbius inversion method is introduced to study the metal/oxide interface. By using this method with a Ni/Al_2O_3 interface, we get a concise and general inversion formula, which helps us to extract interfacial pair potentials from *ab initio* adhesive energies. Now, we talk about its advantages and shortcomings.

There are several advantages with this new general method. First, a concise inversion formula is obtained. It can greatly reduce the effort in theoretical derivations and iterative calculations. Second, the original *ab initio* energies can be precisely reproduced by the inversed potentials. It shows that the inversion formula is self-consistent. Third, these potentials are free-standing pair potentials. They are extracted from *ab initio* adhesive energies directly by a simple iterative calculation, without any supposition of their functional forms.

Besides these advantages, there are also some limitations of this work. The inversed potentials are not totally transferable for a Ni/Al_2O_3 interface, but prefer the Al terminated cases. It is connected with the pair potential approach being a primary approximation of the interfacial system. However, this method is quite practical and we think it can give us a reasonable understanding of the metal/oxide interface, at least on a qualitative scale. Also, the pair potential model needs to be improved to achieve a more transferable potential, with consideration of the charge transfer and many-body interactions on the interface. This is our future work.

Acknowledgments

This work is supported by the Nature Science Foundation of China (NSFC), No. 50531050 and 973 project, No. 2006CB605100. We also express our thanks to H Y Zhao for checking this work.

References

[1] Zhang W, Smith J R and Evans A G 2002 The connection between *ab initio* calculations and interface adhesion measurements on metal/oxide systems: Ni/Al_2O_3 and Cu/Al_2O_3 *Acta Mater.* **50** 3803

[2] Zhang W, Smith J R, Wang X G and Evans A G 2003 Influence of sulfur on the adhesion of the nickel/alumina interface *Phys. Rev.* B **67** 245414
[3] Smith J R and Zhang W 2000 Stoichiometric interfaces of Al and Ag with Al_2O_3 *Acta Mater.* **48** 4395
[4] Shi S, Tanaka S and Kohyama M 2006 First-principles study on the adhesion nature of the α-$Al_2O_3(0001)$/Ni(111) interface *Modelling Simul. Mater. Sci. Eng.* **14** S21
[5] Han X, Zhang Y and Xu H 2003 First-principles calculation on adhesions of Ni/Al_2O_3 and Ni/ZrO2 interfaces *Chem. Phys. Lett.* **378** 269
[6] Jarvis E A A, Christensen A and Carter E A 2001 Weak bonding of alumina coatings on Ni(111) *Surf. Sci.* **487** 55
[7] Dmitriev S V *et al* 2003 Coherency of copper/sapphire interface studied by atomistic simulation and geometrical analysis *Surf. Sci.* **542** 45
[8] Dmitriev S V, Yoshikawa N and Kagawa Y 2004 Misfit accommodation at the Cu(111)/α-$Al_2O_3(0001)$ interface studied by atomistic simulation *Comput. Mater. Sci.* **29** 95
[9] Dmitriev S V *et al* 2004 Atomistic structure of the Cu(111)/a-$Al_2O_3(0001)$ interface in terms of interatomic potentials fitted to *ab initio* results *Acta Mater.* **52** 1959
[10] Dmitriev S V *et al* 2006 Modeling interatomic interactions across Cu/α-Al_2O_3 interface *Comput. Mater. Sci.* **36** 281
[11] Chen N X 1990 Modified Mobius inverse formula and its applications in physics *Phys. Rev. Lett.* **64** 1193
[12] Zhang S and Chen N X 2003 Molecular dynamics simulations for high-pressure induced B1–B2 transition in NaCl by Mobius pair potentials *Modelling Simul. Mater. Sci. Eng.* **11** 331
[13] Hao S Q, Chen N X and Shen J 2002 The space group of $Nd_3Fe_{29-x}Ti_x$: A_2/m or P_{21}/c *Phys. Status Solidi* b **234** 487
[14] Cai J, Hu X Y and Chen N X 2005 Multiple lattice inversion approach to interatomic potentials for compound semiconductors *J. Phys. Chem. Solids* **66** 1256
[15] Long Y, Chen N X and Zhang W Q 2005 Pair potentials for metal–ceramic interface by inversion of adhesive energy *J. Phys.: Condens. Matter* **17** 2045
[16] Long Y, Chen N X and Wang H Y 2005 Theoretical investigations of misfit dislocation in Pd/MgO(001) interface *J. Phys.: Condens. Matter* **17** 6149
[17] Duffy D M, Harding J H and Stoneham A M 1992 Atomistic modelling of the metal/oxide interface with image interactions *Acta Metall. Mater.* **40** S11
[18] Duffy D M, Harding J H and Stoneham A M 1993 Atomistic modelling of metal-oxide interfaces with image interactions *Phil. Mag.* A **67** 865–82
[19] Finnis M W 1992 Metal-ceramic cohesion and the image interaction *Acta Metall. Mater.* **40** S25
[20] Purton J, Parker S C and Bullett D W 1997 Computer modeling of metal-oxide interfaces *J. Phys.: Condens. Matter* **9** 5709
[21] Purton J A *et al* 1999 Comparison of atomistic simulations and pseudopotential calculations of the MgO100/Ag100 and MgO110/Ag110 interfaces *J. Chem. Phys.* **110** 8090
[22] Yao Y G and Zhang Y 1999 *Ab initio* pair potentials at metal–ceramic interfaces *Phys. Lett.* A **256** 391
[23] Endou A *et al* 2000 Potential energy surface and dynamics of Pd/MgO(001) system, as investigated by periodic density functional calculations and classical molecular dynamics simulations *Japan. J. Appl. Phys.* **39** 4255–60
[24] Vervisch W, Motter C and Goniakowski J 2002 Theoretical study of the atomic structure of Pd nanoclusters deposited on a MgO(100) surface *Phys. Rev.* B **65** 245411
[25] Accelrys Inc. *Cerius*^{2} *Users Guide*
[26] Milman V *et al* 2000 *Int. J. Quantum Chem.* **77** 895
[27] Monkhorst H J and Pack J D 1976 Special points for Brillouin-zone integrations *Phys. Rev.* B **13** 5188
[28] Macdonald A H 1978 Comment on special points for Brillouin-zone integrations *Phys. Rev.* B **18** 5897