The atomistic simulation study of Ag/MgO interface tension fracture

X.M. You^a, L.H. Liang^{a,c,*}, Y.G. Wei^{a,b,*}

^a LNM, Institute of Mechanics, Chinese Academy of Sciences, Beijing 100190, China

^b College of Engineering, Peking University, Beijing 100871, China

^c School of Engineering Science, University of Chinese Academy of Sciences, Beijing 101408, China

ARTICLE INFO

Article history:

Received 31 July 2017

Received in revised form 13 October 2017

Accepted 15 October 2017

Available online 6 November 2017

Keywords:

Interface fracture

Stress

Displacement

Molecular simulation

ABSTRACT

Metal/ceramic interfaces have wide applications and the interface fracture plays an important role in determining mechanical behaviors of related structures. The cohesive zone model is widely used to modelling the crack opening and extension, especially used to modelling the interface crack. Although this model is widely used, it is a macroscopic phenomenological model, and its atomistic scale mechanism attracts great attention. In this paper an interface atomistic model of Ag/MgO is used to study the microscopic interface opening mode and some interesting results are discovered. By considering all atomic interaction potentials related to the interfacial structure in the molecular mechanics calculation, the interface tension stress-displacement curves for several interface structures with different sizes are simulated, and fracture properties upon displacing Ag and MgO adjacent to the interface are revealed based on the simulation results and by developing a series model on interface fracture properties. The results indicate that the interface fracture strength is independent of the size of interface structures for ideal interfaces, the total tension displacement of interface structures increases and the fracture appears catastrophic characteristic with increasing unit thickness, which is explained well by the series model. Furthermore, the interface separation behaviors of interfaces with the atomic vacancy and dislocations are simulated, the study indicates that the interface strength decreases for the interfaces with defects, and the defects decrease the catastrophic tendency.

© 2017 Elsevier B.V. All rights reserved.

1. Introduction

Metal/ceramic interfaces have extensive applications in many fields such as catalytic converters, field effect transistors, and anti-corrosion coatings, etc. and play important role in thermal barrier coatings used in aircraft and power generation turbines, thus attract great interest. The interface fracture affects the function of corresponding parts. The cohesive zone model is widely used to study the opening and the extension of the interface crack, and is a macroscopic phenomenological model and a simplification of physical process of the interface fracture at different scales [1–6]. The interface separation stress was expressed as a function of the interface separation displacement in the model, different function forms were used to study the interface fracture in different work groups [1–6]. But we know very little of the microscopic interface opening mode. Recently, the atomic scale simulation of

iron/precipitate interface decohesion was carried out and the cohesive law was discussed [7]. The non-local separation constitutive laws for Cu interface between grains were studied based on molecular dynamic simulations, some internal variables were introduced and damage in the interface was analyzed [8]. However, the atomic scale simulations on metal/ceramic interface separation are few reported due to the difficult of obtaining the potential functions of interface and ceramics.

In this paper, we build a metal/ceramic interface atomistic model to do some researches. Many experimental results of Ag/MgO interfaces have been obtained [9–11]. Moreover, the lattice mismatch between Ag and MgO is small, and the crystal cell size in the calculation is also smaller, thus Ag/MgO interface is a good interface model. The atomistic simulation of Ag/MgO interface tension separation is carried out in this paper by considering all interfacial atomic interaction potentials based on the molecular mechanics calculation and the energy minimization method. Since some defects exist invariably in actual interfaces, we also build the interface model on the imperfect interfaces to study the effects of the vacancy and the dislocations. The intrinsic interface fracture property is revealed by simulating the interface tension stress-displacement curves for the interface structures with different

* Corresponding authors at: LNM, Institute of Mechanics, Chinese Academy of Sciences, Beijing 100190, China. College of Engineering, Peking University, Beijing 100871, China.

E-mail addresses: lianglh@lnm.imech.ac.cn (L.H. Liang), weiyg@pku.edu.cn (Y.G. Wei).

sizes and different defect degrees. The interface fracture strength is found to be independent on the size of the interface structures for ideal interfaces, and the model can be applied to study the separation behavior of the strong adhesive interfaces.

2. Model and methodology

2.1. Interface structure model

We constitute the interface Ag(001)/MgO(001), which is the common interface orientation observed in the experiments [11]. Ag atom is located above O ion, which is the structure with the minimum energy based on the calculation. For convenience, we take 3 Ag and 3 MgO crystal cells in [001] direction that is normal to the interface, and take 5 crystal cells in [100] and [010] directions those are parallel to the interface for Ag and MgO, respectively, which is represented by $5 \times 5 \times 3$, the atom structure is shown in Fig. 1(a). The vacuum layers are inserted above Ag layer and under MgO layer to satisfy three dimensions periodicity, and the interface structure unit with the vacuum layers is built. The atoms in the top and the bottom layers of the interface structure are fixed as shown in Fig. 1(b), and the interface structure unit is also fixed as a representative unit in the whole interface periodic structure. Considering the small mismatch between Ag and MgO, the lattice constants of Ag and MgO are both taken as 4.32 Å (the lattice constant of MgO), since the Ag lattice is easy to be forced to match the more rigid MgO lattice, and the interface distance is

set as 2.4 Å, the thickness of the vacuum layer is 30 Å, the initial structure is thus constituted and then relaxed by the energy minimization calculation. In the calculation, the residual stress rms = 0.01 cal/mol/Å is set, and the maximum iterative times is set as 10000 in the iterative process, the enough small residual stress and enough large iterative times are selected based on the energy minimization by using Smart Minimizer method. The equilibrium interface distance is 2.576 Å after the relaxation, which is in agreement with the experimental result of 2.52 Å [11]. The interface tension fracture process is divided into a series of medium steps, and each step is studied using an energy minimization program by a Cerius² software provided by Accelrys company, the tension process is approximately quasi-static process.

The interface tension is performed by applying a same small displacement normal to the interface on every atom in the top layer of Ag, i.e., the metal is stretched and the ceramic is fixed. The ceramic is stretched and the metal is fixed, or the metal and the ceramic are both stretched, the same results can be obtained, which has been proved by our calculation. The inner stress of the system is calculated at the relaxation state after the enforced tension and the energy minimization in each step, the corresponding interface equilibrium structure is recorded at the same time. Combining all steps, the interface separation process can be described. In every tension, the displacement is set as 0.03 Å. The interface inner stress is calculated according to the outmost layer of the metal atoms or the ceramic atoms since the stress of the fixed atoms is not zero unlike the inner movable atoms. Also, the stress parallel to the interface is small and negligible, thus only the stress normal to the interface is calculated. The interface stress σ is expressed as

$$\sigma(h) = \frac{\sum_{i=1}^n f_i}{S}, \quad (1)$$

where $h = L_2 - L_1$ is the total tension displacement of the interface structure with L_2 and L_1 being the respective total thickness of the interface structure after and before the tension as shown in Fig. 1(b), n is the atomic number of the outmost layer of the metal or the ceramic, f_i is the force applied on the atom i by the other atoms, S is the interface area. The stress value based on Eq. (1) is the same as that based on the energy difference method.

2.2. Interface atomic potentials

In the calculation, a pair potential is taken as the interatomic potential that gives an energetic description of the target system, and the potential is obtained by the Chen-Möbius inversion method based on the *ab initio* calculation [12–14]. The approach has been proved to be practical and reasonable for the interface systems [13]. Ag/MgO interface contains several kinds of interatomic potentials: the metal-oxide terms $\Phi_{\text{Ag-O}}$ and $\Phi_{\text{Ag-Mg}}$, the metal-metal term $\Phi_{\text{Ag-Ag}}$, and the oxide-oxide terms $\Phi_{\text{O-O}}$, $\Phi_{\text{Mg-Mg}}$ and $\Phi_{\text{Mg-O}}$. The potential function across the interface $\Phi_{\text{Ag-O}}$ and $\Phi_{\text{Ag-Mg}}$ refers to the modified Rahman-Stillinger-Lemberg (RSL2) potential [13],

$$\Phi = D_0 e^{\gamma \left(1 - \frac{r}{r_0}\right)} + \frac{a_1}{1 + e^{b_1(r-c_1)}} + \frac{a_2}{1 + e^{b_2(r-c_2)}} + \frac{a_3}{1 + e^{b_3(r-c_3)}}, \quad (2)$$

where r is the interfacial atomic distance, the other parameters are the interface potential parameters referred to Table 1. The ionic interaction potentials $\Phi_{\text{O-O}}$, $\Phi_{\text{Mg-Mg}}$ and $\Phi_{\text{Mg-O}}$ include two parts: the long-range Coulomb interaction potential Φ^{Coul} and the short-range potential Φ^{SR} [15]. The Coulomb term is determined by the effective charge $2e$,

$$\Phi_{\text{Mg-Mg}}^{\text{Coul}} = \Phi_{\text{O-O}}^{\text{Coul}} = -\Phi_{\text{Mg-O}}^{\text{Coul}} = \frac{Q_{\text{eff}}^2}{4\pi\epsilon_0 r} \quad (3)$$

Fig. 1. (a) The atomic structure schematic of the interface, and (b) the interface tension schematic.

Table 1

The potential parameters in Eqs. (2) and (4).

Atomic pairs	Potential parameters		
$\Phi_{\text{Ag-Mg}}$	$D_0 = 284.5542$ kcal/mol $a_1 = 1600.6582$ kcal/mol $a_2 = 7.0657$ kcal/mol $a_3 = 71.1797$ kcal/mol	$R_0 = 1$ Å $b_1 = 6.2388$ Å ⁻¹ $b_2 = 3.6581$ Å ⁻¹ $b_3 = 4.3778$ Å ⁻¹	$y = 2.0843$ $c_1 = 1.1478$ Å ⁻¹ $c_2 = 2.9842$ Å ⁻¹ $c_3 = 1.8999$ Å ⁻¹
$\Phi_{\text{Ag-O}}$	$D_0 = 5596.5601$ kcal/mol $a_1 = -5678.4394$ kcal/mol $a_2 = -634.8887$ kcal/mol $a_3 = -7.4067$ kcal/mol	$R_0 = 1$ Å $b_1 = 2.8384$ Å ⁻¹ $b_2 = 2.1121$ Å ⁻¹ $b_3 = 2.5757$ Å ⁻¹	$y = 2.1383$ $c_1 = 1.0839$ Å ⁻¹ $c_2 = 1.9$ Å ⁻¹ $c_3 = 3.5539$ Å ⁻¹
$\Phi_{\text{Ag-Ag}}$	$D_0 = 4760.9502$ kcal/mol $a_1 = -1747.8618$ kcal/mol $a_2 = 7.0657$ kcal/mol $a_3 = -13.0113$ kcal/mol	$R_0 = 1$ Å $b_1 = 2.2129$ Å ⁻¹ $b_2 = 1.4495$ Å ⁻¹ $b_3 = 0.6884$ Å ⁻¹	$y = 1.6171$ $c_1 = 1.6720$ Å ⁻¹ $c_2 = 2.2826$ Å ⁻¹ $c_3 = 0.9140$ Å ⁻¹
$\Phi_{\text{O-O}}$	$D_0 = 19.9871$ kcal/mol	$R_0 = 2.3600$ Å	$y = 9.4500$
$\Phi_{\text{Mg-Mg}}$	$D_0 = 19.7866$ kcal/mol	$R_0 = 2.4200$ Å	$y = 9.9600$
$\Phi_{\text{Mg-O}}$	$D_0 = 25.2069$ kcal/mol	$R_0 = 2.4503$ Å	$y = 5.9832$

with Q_{eff} being the effective charge quantity and ϵ_0 being the dielectric constant. The short-range term $\Phi_{\text{O-O}}^{\text{SR}}$ and $\Phi_{\text{Mg-Mg}}^{\text{SR}}$ refers to the Morse potential,

$$\Phi = D_0 \left[e^{\gamma \left(1 - \frac{r}{R_0} \right)} - 2e^{\frac{\gamma}{2} \left(1 - \frac{r}{R_0} \right)} \right]. \quad (4)$$

The short-range term $\Phi_{\text{Mg-O}}^{\text{SR}}$ is exponential decay form as the first term in Eq. (2). The metal atomic interaction potential also refers to the RSL2 potential as Eq. (2). All potential parameters are in Table 1.

To test the reliability of selected potential for bulk materials, the lattice constants of Ag and MgO under zero temperature and zero pressure are calculated based on the above potentials, which are agreeing with the experimental results [16] as shown in Table 2. In fact, the elastic constants are also calculated to compare with the experimental results as shown in Table 2, the approximate agreement is also found and the error is about 3–8% for C_{11} and C_{12} . The error for C_{44} is larger, but which is reasonable based on the limitation of the pair potential, and which is not paid attention since the deformation normal to the interface is discussed for the interface tension.

3. Results and discussions on ideal interfaces

3.1. Different interface area

Fig. 2 shows the simulation results of the interface tension for the interface structures with four different interface areas and the same unit thickness. The interface area, i.e., the area of the cross-section, is represented by the number of the crystal cells parallel to the interface, and the unit thickness is represented by the number of the crystal cells normal to the interface. The results indicate that the tension stress σ increases firstly with increasing total tension displacement h of the interface structure unit, then decreases after up to the maximum stress σ_{max} (equal to the inter-

face fracture strength approximately), vanishes finally when the interface separates completely as shown in Fig. 2(a). The interface area has no influence on the results, and four σ - h curves are overlapping. Fig. 2(b) shows the interface opening displacement δ , $\delta = r_2 - r_1$ with r_2 and r_1 being the respective interface atomic distance after and before the tension, versus the total tension displacement h of the interface structure for four corresponding interfaces. It can be seen that δ increases slowly with increasing h firstly, then increases suddenly at h corresponding to the interface strength, i.e., appears jump rise, after that increases slowly again. The jump of δ indicates the catastrophic fracture of the interface. The interface area has no influence on the δ - h curves, too.

3.2. Different unit thickness

Fig. 3 shows the simulation results of the interface tension for the interface structures with seven different unit thicknesses and the same interface area. It can be seen from Fig. 3(a) that the interface fracture strength σ_{max} is a constant for different sizes of the interface structures, but the stress σ drops faster after up to σ_{max} with increasing unit thickness, i.e., the fracture tends to be catastrophic. The total tension displacement h of the interface structure corresponding to σ_{max} increases with increasing unit thickness, i.e., the unit structure is stretched longer for the thicker interface structure, which agrees with Nguyen and Ortiz's discussion [17]. Fig. 3(b) shows δ - h curves of seven corresponding interface structures, the result also indicates that the interface opening tends to be catastrophic fracture with increasing unit thickness.

Fig. 3(c) shows σ - δ curves of seven corresponding interfaces, and all σ - δ curves are overlapping despite of different interface sizes, which implies that the interface tension fracture properties (the fracture strength, the fracture toughness- the area under the σ - δ curve, and the fracture displacement δ_{max}) are intrinsic properties of the interface with the same components, and the interface fracture properties are independent on the size of the systems. The shape of σ - δ curves of Ag/MgO based on our molecular

Table 2

The comparison of the lattice constant a and elastic constants C_{11} , C_{12} and C_{44} of bulk materials between the present calculation based on the potential parameters in Table 1 and the experimental results [16].

		a (Å)	C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)
Ag	This work	4.108	131.998	85.134	85.139
	Expt.	4.086	122.2	90.7	45.4
MgO	This work	4.32	319.2	89.9	89.9
	Expt.	4.22	294	93	155

Fig. 2. (a) The interface tension stress σ versus the total tension displacement h , and (b) the interface opening displacement δ versus the total tension displacement h for four interface structures with different interface areas.

mechanics calculation is in agreement with that of Ni/Al₂O₃ based on the first principle calculation [18] and the usual form of the cohesive zone model [5], although the interface fracture strength, the toughness and the displacement are different for Ni/Al₂O₃ and Ag/MgO interfaces. Therefore, the interface model based on the molecular mechanics can be applied to study the separation behavior of the strong adhesive interfaces.

3.3. The theoretical explanation by developing a series model

The interface system includes three parts: the metal with the thickness L_m and the Young's modulus E_m , the ceramic part with the thickness L_c and the Young's modulus E_c , and the interface part with the distance r as shown in Fig. 1(b). Assuming that the metal and the ceramic part are elastic parts, and the interface is a damage part obeying the stress (σ_i) - displacement (δ_i) relation as shown in Fig. 3(c). The whole system is in equilibrium during quasi-static tension process, and the cross-sections of three parts are equal, the stress in each part is equal,

$$\sigma_m = E_m \varepsilon_m = \sigma_i = E_c \varepsilon_c = \sigma_c, \quad (5)$$

where σ_m and ε_m are the stress and the strain of the metal in the quasi-static tension process, σ_c and ε_c are the stress and the strain of the ceramic part. The total displacement of the system $h = u_m +$

Fig. 3. (a) σ versus h , (b) δ versus h , and (c) σ versus δ for seven interface structures with different interface thicknesses.

$\delta_i + u_c = L_m \varepsilon_m + \delta_i + L_c \varepsilon_c$ is the sum of that of three parts with u_m and u_c being the displacement of the metal and the ceramic part, respectively, combining with Eq. (5),

$$h = \left(\frac{L_m}{E_m} + \frac{L_c}{E_c} \right) \sigma_i + \delta_i. \quad (6)$$

The system deforms continuously with loading firstly, when the released elastic energy of the metal and ceramic parts can counteract the dissipated energy of the interface due to its deformation and damage, the interface will fracture catastrophically, and the

system transformed into a new equilibrium state from the initial equilibrium state. Otherwise, the system will keep quasi-continuous deformation until losing the strength completely. The critical condition of the interface catastrophic fracture is

$$\frac{dh}{d\delta_i} = 0, \quad (7)$$

i.e., an infinite small increment of controlling displacement will lead to a finite response of damage [19], and the damage part cannot keep continuous deformation any more, thus the interface displacement increases abruptly and the interface fracture catastrophically. According to the critical condition of the elasticity instability, the catastrophic point can be derived as

$$\frac{dh}{d\delta_i} = \left(\frac{L_m}{E_m} + \frac{L_c}{E_c} \right) \frac{d\sigma_i}{d\delta_i} + 1 = 0 \quad (8)$$

based on Eq. (6). Therefore,

$$\frac{d\sigma_i}{d\delta_i} = -\frac{E_c E_m}{L_m E_c + L_c E_m}. \quad (9)$$

Eq. (9) shows the slope of stress change is negative, which means the catastrophic point is a point after the maximum stress. When L is larger, the slope is larger, the catastrophic point is more close to the maximum stress point, i.e., the catastrophic characteristic is more obvious for the thicker interface structure, which is in agreement with the simulation results.

The total released energy U_t of the system resisting tension, including elastic strain energy U_e of the metal and ceramic part and interface dissipation energy U_i , can be calculated based on Eqs. (5) and (6),

$$U_t = \sigma_i \frac{h}{L_1} = \frac{\sigma_i}{L_1} \left[\left(\frac{L_m}{E_m} + \frac{L_c}{E_c} \right) \sigma_i + \delta_i \right] = U_e + U_i, \quad (10)$$

where $L_1 = L_m + L_c + r_1$ is the initial thickness of the whole interface structure. For different systems at the maximum stress σ_{ic} point, U_e is almost a constant based on Eq. (11) since σ_{ic} is a constant for different thicknesses as shown in Fig. 3(a), and $U_i = \sigma_{ic} \delta_{ic} / L_1$ decreases with increasing L_1 , since $\sigma_{ic} \delta_{ic}$ (related to interface fracture toughness) is a constant as shown in Fig. 3(c) with δ_{ic} being the critical interface displacement corresponding to σ_{ic} , which means the interface contribution decreases relatively for the thicker unit structures. Combining with the simulation results of the stress and displacement (strain) from Fig. 3(a) and (c), U_i and U_e can be calculated as shown in Table 3. It can be seen from Table 3 that the elastic energy of the metal and ceramic part is smaller than the interface energy contribution for $5 \times 5 \times 2$ interface structure, and larger than the interface energy contribution for the structures thicker than $5 \times 5 \times 3$, which is in agreement with the above discussion on the energy condition of catastrophic characteristic, the fracture of the structures thicker than $5 \times 5 \times 3$ is catastrophic, but the fracture for the structures thinner than $5 \times 5 \times 3$ is continuous as shown in Fig. 3(a).

Note that the united unit GPa is used when the energy is discussed, when the unit is transformed to be J/m² by multiplying the thickness of interface structure, the stable interface energy is about 0.19 J/m² except the thinnest structure. While the elastic energy increases with increasing thickness with changed unit and is 0.22 J/m² for $5 \times 5 \times 3$ structure at the transformed point

of fracture characteristic, so the total released energy is 0.41 J/m² based on Eq. (11), which is equal to the intrinsic interface fracture energy, i.e., the area under the interface stress-interface displacement curve as shown in Fig. 3(c). Therefore, the interface properties of the interface structure at the transformed point of fracture characteristic can be selected as a reference.

Furthermore, assuming the catastrophic point is the point of maximum stress, which is reasonable for larger L , the total displacement of the system at the catastrophic point can be obtained in terms of Eq. (6),

$$h_c = \left(\frac{L_m}{E_m} + \frac{L_c}{E_c} \right) \sigma_{ic} + \delta_{ic}. \quad (11)$$

Eq. (11) indicates the total displacement is larger for larger L , i.e., the thicker interface structure can be stretched longer, which also agrees with the simulation results. Since the interface atomistic model is intrinsic for the interface fracture properties of a system despite of the size, the property of the thicker system can be obtained by the interface atomistic model for the thinner system combining with Eq. (11), which can decrease the computation time and cost.

4. The interfaces with defects

4.1. The interfaces with atomic vacancy

Considering the defects in real materials and interfaces, the tension fracture behavior of the interface with part atomic vacancy is further simulated. The atoms in the bottom layer of Ag of the ideal interface are deleted partly randomly, the vacancy ratio is defined as a ratio of the number of vacancy to the total number of atoms in the bottom layer of Ag of the ideal interface. The calculation indicates that different random vacancy distributions with the same vacancy ratio have no influence on the results.

Fig. 4 shows the results of eight different vacancy ratios for $8 \times 8 \times 6$ interface structures, the results indicate that the interface fracture strength decreases linearly and the interface opening becomes smooth and continuous with increasing vacancy ratio (Fig. 4(a)–(c)). The different interface area has still no influence on the results. The effects of different unit thickness with the same vacancy ratio on the interface strength and the interface opening are the same as those for the ideal interface structures shown in Fig. 3. Fig. 4(c) shows that the model for the ideal interfaces is not appropriate for the interfaces with the defects, the interface fracture strength is dependent on the defect degree of the interface.

4.2. The interfaces with dislocations

Different from the ideal interfaces and the interfaces with atomic vacancy, [1 1 0] and [1–10] directions are selected to be parallel to the interface for the interface with dislocations considering the smaller atomic number in the minimum periodic unit in this interface structure since the larger interface area will be taken for convenience of introducing dislocations [20]. An extra atomic layer of Ag is inserted along (1 1 1) face of the metal as shown in Fig. 5, i.e., the dislocation line lies in Ag atomic layer neighbor to the ceramic part at the interface, and the burgers vector $B = 1/2$

Table 3
The interface energy contribution and elastic strain energy of the interface structure.

	$5 \times 5 \times 2$	$5 \times 5 \times 3$	$5 \times 5 \times 4$	$5 \times 5 \times 6$	$5 \times 5 \times 10$	$5 \times 5 \times 15$	$5 \times 5 \times 20$
U_i (GPa)	0.11	0.072	0.054	0.036	0.022	0.014	0.011
U_e	0.086 GPa

Fig. 4. (a) σ versus h , (b) δ versus h , and (c) σ versus δ for $8 \times 8 \times 6$ interface structures with eight different atomic vacancy ratios.

[1 1 0]. This structure is the dislocation structure with the minimum energy, and the experiment also observed this dislocation structure [21]. 33 crystal cells of Ag and MgO are taken in [1 1 0] direction, which determines the dislocation density, i.e., the number of crystal cells between two neighbor dislocation lines. 3 crystal cells of Ag and MgO are taken in [1-10] direction, and 3 crystal cells of Ag and 3 crystal cells of MgO are respectively taken normal to the interface, i.e., $33 \times 3 \times 3$ interface structure is established.

Fig. 5. The atomic structure schematic of the interface with the dislocation.

Fig. 6. σ versus h of the interface structures with dislocations and the corresponding ideal interfaces with four different interface thicknesses.

Fig. 6 shows the simulation results of the interface tension for four different interface thicknesses with the same dislocation density. The results indicate that the interface fracture strength decreases with increasing unit thickness due to the introducing of the dislocations, and the interface opening still tends to be catastrophic fracture with increasing unit thickness. Comparing with the corresponding ideal interfaces, the interface strength decreases obviously and the total tension displacement also decreases. The strength decrease is due to the extra energy of the defects actually, and the total released energy of the interface structures with dislocations decreases compared to with that of the ideal interfaces, the average total energy difference, i.e., the area difference under the stress-displacement curves as shown in Fig. 6, is about 0.14 Jm^{-2} , which corresponds to the dislocation strain energy and is in agreement with the calculation results of the dislocation energy ($0.1\text{--}0.2 \text{ Jm}^{-2}$) for similar metal/ceramic interfaces [20]. In fact, if the real mismatch between Ag and MgO, with the mismatch strain of

Fig. 7. The atomic structure change image in the interface tension process for $33 \times 3 \times 3$ interface structures without the dislocation (a)–(d) and with the dislocation (e)–(h) and the corresponding σ – h curves.

about 3%, is considered, the mismatch strain energy is about 0.08 – 0.24 Jm^{-2} depending on the thickness based on the related interface strain energy model [22], which agrees with present results.

On the other hand, the interface opening for the interface with dislocations initiates from the dislocation core, different from that for the ideal interface, which can be observed in the interface atomic structure change process simulation as shown in Fig. 7. Fig. 7((a)–(d)) show the whole interface is broken at the same time for the ideal interfaces, and the interface is broken gradually from the dislocation core for the dislocation interface as shown in Fig. 7 ((e)–(h)).

5. Conclusions

A simple interface model of metal/ceramic interface is developed to study interface tension fracture behavior based on the molecular mechanics method and the appropriate interface atomic potentials, and a series model on the interface fracture properties for ideal interfaces is developed, which can be used to explain the separation behavior of the interface structures with different thicknesses. The interface tension stress-displacement curves for different interface structures are simulated, and the intrinsic interface fracture properties are discovered. The results indicate that the interface fracture strength is a constant for ideal interfaces, but decreases with increasing defect degrees; the interface structure is stretched longer and the interface opening becomes catastrophic fracture with increasing unit thickness for the ideal interfaces, but the interface opening becomes continuous with increasing vacancy ratio, the fracture initiates from the dislocation core and the total tension displacement decreases for the interface structures with dislocations.

On the other hand, the interface shear also contributes to the interface fracture, the point is not considered in this paper, which will be discussed in next work. Note that the interface separation characteristics of Ag/MgO in this paper are not particular, in fact we simulated Ni/Al₂O₃ interface and the similar results can be obtained. The work is hopeful to help understanding the intrinsic

interface fracture mechanism of metal/ceramic interface used in thermal barrier coatings. Certainly, temperatures will affect interface separation behaviors more or less, and the temperature effect can be further studied by the molecular dynamics method in next work.

Acknowledgements

The work is supported by the Research Grants from NSFC through grant nos. 11372318, 11672296, 11432014, 11672301, and the Strategic Priority Research Program of the Chinese Academy of Sciences (Grant No. XDB22040501).

References

- [1] G.I. Barenblatt, The mathematical theory of equilibrium of cracks in brittle fracture, *Adv. Appl. Mech.* 7 (1962) 55–129.
- [2] D.S. Dugdale, Yielding in steel sheets containing slits, *J. Mech. Phys. Solids* 8 (1960) 100–104.
- [3] A. Needleman, An analysis of decohesion along an imperfect interface, *Inter. J. Fract.* 42 (1990) 21–40.
- [4] V. Tvergaard, J.W. Hutchinson, The relation between crack growth resistance and fracture process parameters in elastic-plastic solids, *J. Mech. Phys. Solids* 40 (1992) 1377–1397.
- [5] Y.G. Wei, J.W. Hutchinson, Toughness of Ni/Al₂O₃ interfaces as dependent on micron-scale plasticity and atomistic-scale separation, *Phil. Mag.* 88 (2008) 3841–3859.
- [6] Y.G. Wei, Modeling nonlinear peeling of ductile thin films-critical assessment of analytical bending models using FE simulations, *Int. J. Sol. Struc.* 41 (2004) 5087–5104.
- [7] A. Elzas, B. Thijssse, Cohesive law describing crack growth at iron/precipitate interfaces, *Comp. Mater. Sci.* 134 (2017) 214–224.
- [8] D.E. Spearot, K.I. Jacob, D.L. McDowell, Non-local separation constitutive laws for interfaces and their relation to nanoscale simulations, *Mech. Mater.* 36 (2004) 825–847.
- [9] E. Pippel, J. Woltersdorf, J. Gegner, R. Kirchheim, Evidence of oxygen segregation at Ag/MgO interfaces, *Acta Mater.* 48 (2000) 2571–2578.
- [10] J. Hosson, B. Kooi, B. J. Metal-ceramic interfaces: a microscopic analysis, *Surf. Interface Anal.* 31 (2001) 637–658.
- [11] O. Robach, G. Renaud, A. Barbier, Structure and morphology of the Ag/MgO (001) interface during in situ growth at room temperature, *Phys. Rev. B* 60 (1999) 5858–5871.
- [12] N.X. Chen, Modified Möbius inversion formula and its application in physics, *Phys. Rev. Lett.* 64 (1990) 1193–1195.

- [13] Y. Long, N.X. Chen, W.Q. Zhang, Pair potentials for a metal-ceramic interface by inversion of adhesive energy, *J. Phys.: Condensed Matt.* 17 (2005) 2045–2058.
- [14] Y. Long, N.X. Chen, Pair potential approach for metal/ Al_2O_3 interface, *J. Phys.: Condensed Matt.* 19 (2007) 196216.
- [15] S. Zhang, Ionic Interaction Potential by Lattice Inversion Ph. D Thesis, Tsinghua University, 2002.
- [16] M. Levy, H.E. Bass, R.R. Stern, *Handbook of Elastic Properties of Solids, Liquids, and Gas V. 2*, Academic Press, 2000.
- [17] O. Nguyen, M. Ortiz, Coarse-graining and renormalization of atomistic binding relations and universal macroscopic cohesive behavior, *J. Mech. Phys. Solids* 50 (2002) 1727–1741.
- [18] J.R. Smith, Y. Jiang, A.G. Evans, Adhesion of the $\gamma\text{-Ni(Al)}/\alpha\text{-Al}_2\text{O}_3$ interface: a first principles assessment, *Int. J. Mat. Res.* 98 (2007) 1214–1221.
- [19] S.W. Hao, M.F. Xia, F.J. Ke, Y.L. Bai, Evolution of localized damage zone in heterogeneous media, *Int. J. Damage Mech.* 19 (2010) 787–804.
- [20] Y. Long, N.X. Chen, Atomistic simulation of misfit dislocation in metal/oxide interfaces, *Comp. Mater. Sci.* 42 (2008) 426–433.
- [21] G. Renaud, P. Guenard, A. Barbier, Misfit dislocation network at the Ag/MgO (001) interface: A grazing-incidence x-ray-scattering study, *Phys. Rev. B* 58 (1998) 7310–7328.
- [22] G. Ouyang, L.H. Liang, C.X. Wang, G.W. Yang, Size-dependent interface energy, *Appl. Phys. Lett.* 88 (2006) 091914.