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A molecular dynamics based cohesive zone model for predicting interfacial properties between graphene coating and aluminum



Wu-Gui Jiang^{a,b,*}, Yao Wu^a, Qing-Hua Qin^c, Duo-Sheng Li^d, Xiao-Bo Liu^a, Ming-Fu Fu^b

^a School of Aeronautical Manufacturing Engineering, Nanchang Hangkong University, Nanchang 330063, China

^b Gongqing Institute of Science and Technology, Jiujiang 332020, China

^c Research School of Engineering, The Australian National University, Acton, ACT 2601, Australia

^d School of Materials Science and Engineering, Nanchang Hangkong University, Nanchang 330063, China

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ABSTRACT

A cohesive zone model (CZM) based on a traction–separation (T-S) relation is first developed to simulate the interfacial behavior between graphene coating and aluminum (Al) substrate. The CZM parameters, which are very difficult to obtain directly experimentally, are determined using molecular dynamics (MD) simulation. Specifically, the MD simulations under the normal and shear loadings are conducted on the graphene-coating/Al interface to derive its T-S relation and then the relevant interfacial behavior of the composite is identified. The MD results show that the behavior of the interface between graphene coating and Al substrate under normal and shear loading is temperature dependent. The maximum normal tensile stress at the interface decreases gradually while the temperature increases from 150 K to 600 K. But the maximum shear stress increases as the temperature increases from 150 K to 450 K and then decreases as the temperature increases from 450 K to 600 K. Finally, the CZM parameters are determined and then imported into a finite element (FE) model. The blister test results suggest that the proposed approach is efficient in determining the CZM parameters of the interfacial behavior between the substrate and the ultrathin coating.

1. Introduction

Though graphene has a Young's modulus of 1.1 TPa and a high intrinsic strength of 125 GPa, its independent use as a structural material is still problematic because it is a two-dimensional crystal of atomic thickness [1]. In contrast, aluminum is widely used as a strengthening structural material because of its high specific strength and light weight. Graphene fragments, as a promising strength enhancer in composites [2], have been demonstrated to improve the strength and toughness of composites, even without ordered arrangements [3,4]. On the other hand, Al always severs in a complex environment. Coating is a popular way to protect the Al products. Recently, Kirkland et al. [5] reported that, compared with alumina coatings, graphene coatings possess many unique properties that are especially suitable for the lightest and thinnest protective barriers of metal components, due to their excellent electrical conductivity, heat resisting property, chemical inertness, and transparency. Chemical vapour deposition (CVD) can produce high-quality graphene films on a metal (for example, Cu, Ni, Pt or alloy) surface at high temperatures, and the films are then transferred to other substrates [6]. It should be noticed that a chemical reaction between Al and graphene can lead to the formation of Al carbide (Al_4C_3) at a higher temperature, which weakens the mechanical properties of graphene-Al composites [7]. So the graphene can be coated on Al surface by using the transferring method.

Many studies have investigated the mechanical properties of graphene/metal nanolayered composites [8-13]. The high intrinsic strength and modulus of graphene dispersed into a metal can effectively constrain dislocation movement in the metal, significantly strengthening the metal. However, graphene-reinforced metal composites exhibit strong interfacial effects under a variety of load conditions. Liu et al. used a molecular dynamics (MD) method to investigate the interfacial strengthening and self-healing mechanism of graphene/copper nanocomposites under shear loading [14]. The interfacial behavior between the graphene and the matrix, especially in the case of a graphene coating on the matrix, plays a significant role in determining the mechanical properties of graphene/matrix composites. In existing finite element (FE) simulations of such composites at micro scale, the interface was often modeled by a cohesive zone model (CZM) in which a traction-separation (T-S) relation between the matrix and the reinforcement phase was employed to describe the matrix/reinforcement

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^{*} Corresponding author at: School of Aeronautical Manufacturing Engineering, Nanchang Hangkong University, Nanchang 330063, China. *E-mail address:* jiangwugui@nchu.edu.cn (W.-G. Jiang).

interaction. However, the cohesive zone law is not universal, and it takes different forms for different material interfaces. Traditionally, the CZM parameters have usually been determined by the quantitative T-S relation that was often obtained from experiments [15,16]. Yet it is very difficult to conduct corresponding experiments with a graphene coating on a matrix. Moreover, the high expense of experimental methods as well as the effect of factors such as lattice mismatch, thermal expansion coefficient mismatch, and crystal defects on the experimental results leads to scattered experimental data and low efficiency. Alternatively, CZMs have been replaced by numerical or analytical modeling of fracture processes. A macroscopic cohesive method introduced by Needleman [17] has been widely used to describe the cohesive zone type interface model, and recently, a modified T-S rule was proposed by Sazgar and Movahhedy [18] to take account of the temperature effect. On the other hand, at atomic scale, MD simulations have been used to predict interfacial behavior between particles and matrix. Gall et al. were the first to obtain the T-S relation by atomistic simulations, when investigating atomic debonding in a silicon/aluminum interface [19]. Subsequently, numerous MD studies were used to investigate the deformation and fracture behavior of single crystal metals such as Al, Cu, Ni, Fe, Cr, W [20], and bi-crystal Al [21,22] under tensile loading. Besides, many MD simulations have been used to study interfacial behavior between two different materials [23-26]. Recent attention has been paid to a multi-scaled CZM. For instance, Dandekar used the local values from MD simulation to derive the global T-S relation for an Al/ SiC interface, and imported the resulting higher scaled CZM parameters to the FE model [27]. Sazgar and Movahhedy [18] developed an MDbased modified Needleman CZM for the prediction of equivalent temperature-dependent material behavior in an Al/Al₂O₃ composite. Comparison of MD simulations and experimental results [18,27] demonstrated the effectiveness of the MD-based CZM approach. Near room temperature, however, graphene has a negative coefficient of thermal expansion (CTE), and the absolute values of the CTEs of graphene first increase and then decrease with increasing temperature in range of 0 K to 600 K [28]. The changing trend of the CTEs of graphene with temperature change is completely unlike the behavior of metal, leading to curious interfacial properties when graphene is coated on metal. Research on this anomaly is still unexplored.

On the basis of the abovementioned research, MD and theoretical analysis are used in this work to study the interfacial behavior of graphene coating on substrate Al under tensile and shear loadings. Then, the Lennard-Jones (LJ) potential function is applied to estimate the quantitative T-S relation used in the CZM model, after which the relevant CZM parameters are imported into the FE simulations to investigate the deformation of graphene coating on the substrate Al. Finally, to verify the proposed method, the blister test, a well-known method for measuring the adhesion of thin films to their substrate, is simulated by using both the FE method with the CZM parameters from the proposed approach and the MD method.

2. Methods and models

In this study, a monolayer graphene is coated on substrate aluminum. It is well known that the in-plane Young's moduli of graphene are very strong, whereas the out-of-plane Young's moduli are quite weak [29]. Therefore, the effect of the chirality of graphene is ignored because of the weak out-of-plane interaction between the coating and substrate. The typical (1 0 0) and (1 1 1) stacking planes of substrate Al are taken into account for investigating the interfacial behavior between the graphene coating and the substrate Al. The two crystal orientation planes of aluminum and graphene are shown in Fig. 1a. Thus, there are two assemblies of graphene-coating/Al composites (GA) with different crystal stacking between the graphene and aluminum layers: graphene-Al (1 1 1) (GA1 1 1) and graphene-Al (1 0 0) (GA1 0 0). To arrive at an acceptable size, various dimensions for the simulation box along the directions with periodic boundary conditions and free boundary conditions are examined, and finally the dimensions of $196.8 \times 42.6 \times 201.71$ Å are obtained for the simulation box. During the tension process, the boundary in *z*-direction is set as free, and the boundaries in *x*- and *y*-directions are set periodic. While during the shear process, the boundaries in *x*- and *z*-directions are set as free, and the boundary in *y*-direction is set periodic. The graphene is set as a rigid body while applying tensile or shear loadings in our simulations, and this setup has been used by Xu and Buehler [30] to calculate the binding energy of graphene/metal via the first-principle method. Fig. 1b shows the initial configuration of the MD simulation built within the MD package of a Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) [31].

The interactions between carbon atoms are described by the adaptive intermolecular reactive empirical bond order (AIREBO) potential [32,33], and those between aluminum atoms are described by an embedded atom model (EAM) [34-36]. Because aluminum and carbon atoms near the interface do not form chemical bonds in the transferring process, the Lennard-Jones (LJ) 12-6 potential is used to describe the interactions of carbon/aluminum [37], which is rather useful in describing the adhesive interface between different components than the Morse potential [27]. The LJ interaction is written as $U_{LJ}(r_{ij}) = 4\varepsilon[(\sigma/$ $r_{ii}^{12} - (\sigma/r_{ii})^6$ ($r_{ii} \leq r_c$) [38,39], where r_{ii} is the distance between those atoms not forming bonds, ε is the well depth, σ is the size parameter, and r_c is the cutoff distance. ϵ and σ are 0.03507 eV and 3.0135 Å, respectively [40,41]. The cutoff distance r_c should be taken to be 3 σ or greater, as recommended in [41], so here we employ a cutoff distance of 9.0405 Å in our simulations. Initially, both aluminum and graphene are kept in contact along the interface in the *x*-*z* plane with a separation distance of 3.014 Å. The initial interface separation distance is chosen to be close to the equilibrium bond length of Al-C. The equilibrium bond lengths from ab initio calculations and experiments for the Al-C are in the range of 2.31–3.36 Å [35]. Fig. 2 gives the pair distribution function in the GA111 at 300 K, from which it can be seen that, after relaxation, the interface separation distance of the graphene/Al system is measured in the range of 2.37-2.52 Å. This result is consistent with the equilibrium bond length of Al-C. The simulation box is first kept at the constant temperature for 40 ps by Langvin thermostat to permit a reasonably equal partitioning of the kinetic energy at the beginning. Then, the isobaric-isothermal ensemble (NPT) is utilized for 50 ps to maintain a constant temperature and then impose the pressure of 1 bar to obtain the initial physical state of the material. After equilibrium, the load is finally applied to the simulation box to obtain a T-S relationship curve. All simulated time steps are selected as 1 fs.

To apply shear, tensile, and fixed loads to certain atoms, the areas 8 Å thick at the bottom of substrate Al and the graphene layer are considered to be the loading region (regions a, b, and c in Fig. 1), wherein the graphene layer (region a in Fig. 1(c)) is subjected to a tensile force in the z-direction, and to a shear force (region c in Fig. 1(d)) in the x direction. Region **c** in Fig. 1(c) and (d) is fixed during loading. Due to the abrupt change in the velocity of the atom, the uniform stretching of the system keeps the atom free from computational shock [42]. The values of tensile and shear stresses at the interface are obtained by averaging the values of atomic virial stresses in the entire simulation box. In order to reduce or even eliminate the influence due to elastic deformation, the open displacements of the interface are estimated by the mean atomic displacements of the graphene minus those of the three-layer Al atoms closest to the interface (that is, the thickness of a primitive cell of single crystal Al). Atomic quantities are ensemble averaged both in time and space every 100 fs. Visualization is performed using OVITO [43].

3. Results and discussion

3.1. Traction-separation model

Tensile and shear tests are performed to obtain the T-S relationship



Fig. 1. Schematic of (a) in-plane compatibility of lattice for aluminum and graphene layer in GA composites; (b) sizes of the MD model, where dimensions are in angstrom; schematic of (c) tension and (d) shear MD model for GA composites.



Fig. 2. Diagram of the pair distribution function after relaxation in GA111 at 150 K.

curve at the interface. This relationship explains the interfacial behavior between the substrate and graphene coating in the composite under specific loads.

In order to consider the effects of temperature and crystal orientation on the interfacial behavior, MD simulations are conducted for GA1 1 1 and GA1 0 0 at temperatures of 150, 300, 450, and 600 K. σ_{max} and τ_{max} denote the maximum tensile stress and shear stress of

separation, respectively. Fig. 3(a) and (b) shows the T-S curves of GA111 and GA100 respectively under tensile loading, from which it can be observed that the maximum tensile force decreases gradually as the temperature increases. However, the change trend of the maximum shear stress with temperature displays a completely different pattern from that of the maximum tensile stress. Fig. 4(a) and (b) gives the T-S curves of GA111 and GA100 respectively under shear loading. We can see that, as the temperature increases, the shearing force first increases to reach its maximum at 450 degrees, then decreases with the further increase of temperature. This trend with temperature is related to the changing trend of the thermal expansion coefficient of the graphene in the temperature range 0 to 600 K [44]. The interfacial shear stresses are sensitive to the mismatch of the thermal expansion coefficients between the graphene coating and the Al substrate. The maximum tensile and shear stresses are given in Table 1, where it is found that the maximum tensile stresses in GA111 are always greater than those in GA100 at the same temperature, but the trend of the maximum shear stresses is just the reverse. By means of first-principles calculations, the interface tensile strengths of graphene/copper and graphene/nickel along the [111] direction were calculated by Xu and Buehler [30], respectively, 2.92 GPa and 18.70 GPa. In this study, the calculated interface tensile strength of graphene/aluminum along the [111] direction at 150 K is 5.57 GPa, which is between the two above. The cohesive energy ϕ_c can be expressed as a function of the tensile strength $\sigma_{\rm max}$ and the critical displacement δ_c corresponding to the tensile strength, i.e. $\emptyset_c = -e\sigma_{\max}\delta_c$ [45,46], where *e* represents exponent function. The calculated cohesive energy of graphene/aluminum along the [111]



Fig. 3. The T-S relationship under tensile loading for (a) GA111 and (b) GA100 interfaces at different temperatures.

direction at 150 K is -50.19 meV Å $^{-2}$, which is also between -24.81 meV Å⁻² for graphene/copper and -91.33 meV Å⁻² for graphene/nickel predicted by Xu and Buehler [30]. The interface tensile strength of graphene/aluminum is stronger than 4.57 GPa for alumina/ aluminum [18] and 3.3 GPa for SiC/aluminum [27]. We also noted that, the calculated interface shear strength of graphene/aluminum is only about 0.1 GPa, which is far less than 2.93 GPa for alumina/aluminum [18] and 2.2 GPa for SiC/aluminum [27]. The main reason is that, for alumina/aluminum, some oxygen atoms and aluminum atoms near the interface will form covalent bonds where the Reaxff potential is used to describe the interface between alumina and aluminum [18], while for SiC/aluminum, some carbon atoms and aluminum atoms in the vicinity of the interface will form strong chemical bonds, in which the Morse potential is used to describe the interface between SiC and aluminum [27]. The interfacial shear strength of graphene/aluminum obtained in this study is close to that of copper/niobium interface simulated by Wang et al. [47], and greater than 0.04 GPa for the carbonnanotube/silicon interfaces [48].

Regardless of the temperature of the system or the mode of failure, the traction always initially increases to a peak value and decreases to approximately zero when the crack opening becomes large. The simulated maximum separation distance in the normal direction is about 13 ± 1 Å and in the tangential direction it is 55 ± 5 Å. The cohesive energy calculation results are shown in Table 1. The CZM parameters are dependent on the crystal orientation and temperature.



Fig. 4. The T-S relationship under shear loading for (a) GA1 1 1 and (b) GA1 0 0 interfaces at different temperatures.

 Table 1

 The cohesive interfacial parameters obtained from MD results.

Θ(K)	Crystal orientation	$\sigma_{\rm max}$ (GPa)	$\tau_{\rm max}$ (GPa)	E_n (GPa)	$\phi_{\rm c}~({\rm mev}/{\rm \AA}^2)$
150	111	5.57	0.059	413.994	-50.19
150	100	5.53	0.107	566.096	-43.08
300	111	5.20	0.086	448.615	-43.86
300	100	4.90	0.121	463.868	-41.25
450	111	5.10	0.090	391.537	- 47.94
450	100	4.81	0.144	415.200	-46.64
600	111	4.68	0.051	356.872	-36.11
600	100	4.58	0.121	385.999	-36.00

3.2. Cohesive zone model

The CZM explains the relationship between the interface force and the interface opening displacement. In the CZM, the regions of the two overlapping cohesive surfaces are simplified to an original zero-thickness zone. Under a certain loading, the two surfaces separate and the traction between them varies in accordance with a specified T-S law. A suitable solution for the interface behavior in different loading modes can therefore be demonstrated by the CZM. For this purpose, the CZM curve should be obtained by the formulation of the T-S law.

In this study, on the basis of the macroscopic cohesive method introduced by Needleman [17,49] and the modified T-S rule proposed by Sazgar and Movahhedy [18], the CZM of the temperature-dependent graphene/aluminum system is obtained by the results obtained by MD



Fig. 5. Comparison of the modified CZM with the MD result and the CZM model formulated by Needleman [40].

simulation, as given below:

$$T_{(\kappa)} = \sigma_{\max} A e^2 \kappa \exp(-A e \kappa) (1.3 - 0.001\theta)$$
⁽¹⁾

Here, $T(\kappa)$ describes the traction as a function of the dimensionless parameter κ that is defined as:

$$\kappa = \sqrt{(\Delta_n/\delta_n)^2 + (\Delta_t/\delta_t)^2}$$
⁽²⁾

where Δ_n and δ_n are normal separation and maximum separation in the normal mode, and Δ_t and δ_t are tangential separation and maximum separation in the tangential mode, respectively. Thus, a unit value of κ indicates full failure of the interface. Θ stands for temperature (in

Kelvins). *A* is an adjustable dimensionless constant that is set equal to 1.95 by analyzing the MD simulation results.

Fig. 5 shows the results of the T-S curves of normal stresses of GA100 at 300 K and illustrates the results of Sazgar and Movahhedy's CZM model [18], the MD simulation, as well as the CZM model introduced by Needleman [17,49]. This figure shows three different curves crossing each other. From it, we can demonstrate the properness of Needleman's exponential model through the curve similarity between the MD results and the exponential model [17,49]. Moreover, the modified parameterized CZM is found to be closer to the MD results. Therefore, the MD results are used to develop a parametric CZM that can be achieved in the finite element model of graphene/substrate interactions.

The parameters to be used by the CZM can be obtained from the MD simulations. As shown in Table 1, the parameter $T_{(x)}$ is expressed as the maximum traction force and E_n is expressed as elastic stiffness estimated according to the work of Volino et al. [50].

4. Validation of parameterized CZM

The blister test is a well-known method for measuring interfacial behavior between thin films and their substrate, in which stress concentrations are avoided by the application of a uniform pressure. To study the applicability of the CZM proposed in this study, a finite element model of the blister test consisting of an aluminum matrix, a rigid sphere indenter, and graphene-coating, is prepared, as shown in Fig. 6(a). The sizes of this model are chosen as 19.68, 4.26, and 20.17 nm in the *x*, *y*, and *z* directions, respectively. A cylinder void with a radius of 1 nm is located at the center of the substrate Al, and a rigid sphere indenter with a radius of 0.6 nm is applied with the upward speed of 200 m/s in the *z*-axis direction at the temperature of 300 K.



Fig. 6. (a) Initial schematic of FE model for the blister test in GA; (b) deformation schematic of FE model when the interface is fully separated; (c) initial schematic of MD model for the blister test; (d) deformation schematic of MD model when the interface is fully separated.



Fig. 7. Reaction forces with respect to the indenter displacement in both MD and FE models of the blister test for GA111 at 300 K.

Only the blister test of GA111 is considered here. For comparison, similar MD simulations (Fig. 6c) are performed with the same applied speed. Fig. 6(b) and (d) shows the FE and MD numerical results respectively of the blister test, indicating that the FE and MD model have similar deformation configurations during the blister test. The reaction force of the indenter in the FE model, as well as that in the MD model with respect the indenter displacement, are plotted in Fig. 7, from which the excellent agreement between the FE and MD curves can be clearly seen.

5. Conclusions

A hierarchical series of simulations was carried out from atomistic scaled molecular dynamics (MD) analysis to macro-scaled finite element (FE) modeling to investigate the interfacial properties between graphene coating and aluminum (GA). An interfacial cohesive zone model (CZM) was developed based on the traction–separation (T-S) curves simulated from normal tension and shear pulling MD simulations of the GA interface at temperatures of 150 to 600 K.

Our MD simulations showed that the interfacial tensile strength decreased gradually as the temperature increased, but for the interfacial shear strength, as the temperature increased from 150 K to 450 K, the values of the interfacial shear strength first increased and then decreased with the further increase of temperature from 450 K to 600 K. This trend with temperature was related to the change trend of the thermal expansion coefficient of the graphene in the temperature range from 0 to 600 K.

Finally, the above temperature-dependent CZM parameters were determined and then imported into the FE model. A blister test of graphene coated on aluminum was simulated using the macro-scaled FE method and was verified with the full MD results, suggesting that the proposed approach is efficient in determining the CZM parameters of the interfacial behavior between the substrate and the ultrathin coating.

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