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Characterizing the fracture parameters of a graphene sheet using atomistic simulation and continuum mechanics

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ABSTRACT

The fracture behavior of a graphene sheet, containing a center crack (length of $2a$) was characterized based on the atomistic simulation and the concept of continuum mechanics. Two failure modes, i.e., opening mode (Mode I) and sliding mode (Mode II), were considered by applying remote tensile and shear loading, respectively, on the graphene sheet. In the atomistic simulation, the equilibrium configurations of the cracked graphene subjected to applied loadings, before and after the crack extension of $2\Delta a$, were determined through molecular dynamics (MD) simulation, from which the variation of the potential energy and the strain energy release rate of the discrete graphene sheet because of crack extension was calculated accordingly. It is noted that because of the discrete attribute, there is no stress singularity near the crack tip, and thus, the concept of stress intensity factor that is generally employed in the continuum mechanics may not be suitable for modeling the crack behavior in the atomistic structures. For the sake of comparison, the continuum finite element model with the same geometric parameters and material properties as the atomistic graphene sheet was constructed, and the corresponding strain energy release rate was calculated from the crack closure method. Results indicated that the strain energy release rates obtained from the continuum model exhibit good agreement with those derived from discrete atomistic model. Therefore, it is suggested that the strain energy release rate is an appropriate parameter, which can be employed in the atomistic model and the continuum model for describing the fracture of covalently bonded graphene sheet.

1. Introduction

In the theory of linear elastic fracture mechanics (LEFM), stress intensity factor (SIF) and strain energy release rate (SERR) are the two parameters that are generally introduced in modeling the fracture behaviors of a continuum media. The stress intensity factor basically defines the amplitude of stress singularity at the crack tip, providing essential information, such as stresses, strain, and displacement fields, near the crack tip. It was postulated that the onset of crack extension is governed by the local singular stress field near the crack tip (so-called near tip stress field), and thus, the fracture behavior can be described appropriately using SIF. On the other hand, the strain energy release rate is regarded as the measurement of change in strain energy with an infinitesimal crack extension. It was assumed that when the SERR reaches a critical value, the crack begins to propagate. Although the two quantities were developed based on different physical concepts (one is from the local stress/displacement filed, and the other is from energy variation), their applications to fracture mechanics are essentially equivalent in a linear elastic continuum (Anderson, 1995). In other words, the two fracture parameter can be adopted alternatively in predicting the initiation of the crack embedded in a continuum solid. Nevertheless, if the scale is deduced to a nano range, the material system examined is no longer a continuum solid, but a discrete molecular structure. Under this nano scale, it is interesting to explore if the two fracture parameters developed originally based on continuum concept can be extended and applicable to the discrete atomistic structure.

Jin and Yuan (2005b) investigated the macroscopic fracture parameters from both atomistic simulation and the continuum model, indicating that the near-tip stress field calculated from atomistic simulation agrees well with the continuum stress. A similar observation that the local stress near the crack tip can be well described by $1/\sqrt{r}$ dependence was also addressed by Omeltchenko et al. (1997). Miller et al. (1998) examined the Mode I deformation near the crack tip in a single crystal nickel and then computed the critical stress intensity factor, indicating that the atomistic stress beyond the first three lattice spacings from the crack tip is consistent with the elastic $1/\sqrt{r}$ curve. Because of the atomically blunt crack tip, the atomistic stress in the region near the crack tip deviated from the elastic solution (singular stress

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field). The mixed mode crack in a single crystal nano-plate was characterized by Zhou et al. (2009) using quasi-continuum simulation technique. They addressed that the atomic stress fields neighboring the crack tip are also singular and controlled by the atomic stress intensity factor. If the near-tip stress singularity can be validated in the atomistic simulation, the concept of stress intensity factor may be employed to describe the fracture behavior of discrete atomistic structures. In addition to the stress intensity factor, the strain energy release rate for atomistic graphene sheet with center crack was calculated using J-integral approaching with the assumption of nonlinear constitutive relation (Jin and Yuan, 2005a). The critical value of J-integral J_c was introduced to measure the onset of crack extension of graphene sheet.

In this study, the atomistic structures as well as the continuum model of graphene sheet with central crack were established, respectively. In the discrete model, the local stress field near the crack tip was evaluated by using the hardy stress formula (Hardy, 1982; Zimmerman et al., 2004), and the suitability of the stress intensity factor employed to the atomistic structure was thoroughly examined. In addition, the strain energy release rate in the atomistic model was determined using the global energy method and the crack closure method. For the sake of comparison, the continuum graphene model was established, and the corresponding near tip stress field and strain energy release rate were evaluated from the finite element analysis. The fracture parameters suitable for characterizing the atomistic structure and continuum model were of concern.

2. Atomistic simulation

2.1. Construction of atomistic structures of graphene sheet

Graphite structure is constructed by the carbon layers where the carbon atoms are arranged in a hexagonal pattern. The interatomistic distance between the adjacent carbon atoms is 1.42 Å, and the associated atomistic interaction is covalently bonded by SP^2 hybridized electrons, the bond angle of which is 120° to each other (Cho et al., 2007). In order to investigate the mechanical properties of the graphite, the atomistic structures have to be constructed in conjunction with the appropriately specified atomistic interaction. In the description of graphite structure, two kinds of atomistic interactions are normally taken in account: one is bonded interaction, such as the covalent bond, and the other is the non-bonded interaction, i.e., van der Waals and electrostatic forces. Among the atomistic interactions, the covalent bond between two neighboring carbon atoms that provides the building block of the primary structure of the graphite may play an essential role in the mechanical responses. Such bonded interaction can be described using the potential energy that consists of bond stretching, bond angle bending, torsion, and inversion (Rappe and Casewit, 1997). As a result, the total potential energy of the graphite contributed from the covalent bond can be written explicitly as

$$U_{\text{graphite}} = \sum U_r + \sum U_\theta + \sum U_\phi + \sum U_\omega \tag{1}$$

where U_r is a bond stretching potential; U_θ is a bond angle bending potential; U_ϕ is a dihedral angle torsional potential; and U_ω is an inversion potential. For graphite structures under in-plane deformation, the atomistic interaction is mainly governed by the bond stretching and bond angle bending; therefore, the dihedral torsion and inversion potentials that are related to the out-of-plane deformation were disregarded in the modeling. The explicit form for the bond stretching and bond angle bending can be approximated in terms of elastic springs as (Li and Chou, 2003).

$$U_r = \frac{1}{2}k_r(r - r_o)^2 \tag{2}$$

$$U_\theta = \frac{1}{2}k_\theta(\theta - \theta_o)^2 \tag{3}$$

where k_r and k_θ are the bond stretching force constant and angle bending force constant, respectively. The constants $k_r = 93,800 \frac{\text{kcal}}{\text{mole nm}^2}$ and $k_\theta = 126 \frac{\text{kcal}}{\text{mole rad}^2}$ selected from AMBER force field for carbon–carbon atomic-interaction (Cornell et al., 1995) was employed in our molecular simulation. The parameters r_0 and θ_0 represent bond length and bond angle in equilibrium position, which are assumed to be 1.42 Å and 120°, respectively, for the graphite atomistic structures. In general, in addition to the bonded interaction, the non-bonded interaction, i.e., van der Waals and electrostatic forces, has to be considered in the atomistic simulation. However, as compared to the covalent bond, the non-bonded interaction exhibits less contribution on the mechanical properties of graphene sheet; therefore, it was neglected in our current atomistic model.

The center crack of length $2a$ in the graphene sheet was created by eradicating the associated covalent bond so that for the atom pairs across the crack surface, there is no atomistic interaction taking place. The dimension of the graphene sheet with center crack is illustrated in Fig. 1. In order to construct the atomistic structures of cracked graphene sheet with a stress-free state, the modified NPT ensemble with the characteristics of varying simulation box in shape and size (Melchionna et al., 1993) was conducted in the MD simulation at the time increment of 1 fs for 100 ps. Figs. 2 and 3 illustrate the potential energy and stress histories during the simulation, respectively. It can be seen that after the minimum potential energy is attained, the stress components are also approaching zero. Subsequently, the loading, i.e., uniaxial tensile stress and pure shear stress, was applied respectively on the boundary of graphene sheet to simulate the Mode I and Mode II fracture behaviors. After the modified NPT ensemble (Melchionna et al., 1993) with time increment at 1 fs for 100 ps was performed, the atomistic configuration of graphene sheet with the applied loading was determined. It should be mentioned that in the modified NPT, the stress components could be applied independently on the simulation box; however, in the original NPT, only hydrostatic stress can be implemented on the surfaces of the simulation box. The stress history in the modified NPT ensemble is presented in Fig. 4 where tensile stress (2 GPa) is applied on the graphene sheet to simulate the Mode I fracture. It is noted that in the study, the DL-POLY package originally developed by Daresbury Laboratory (Smith and Forester, 2001) was modified to simulate the uniaxial loading/pure shear loading on the graphene sheet.

2.2. Local stress field near the crack tip

It is well-known that in the continuum media, the square root stress singularity occurs near the crack tip, and thus, the concept

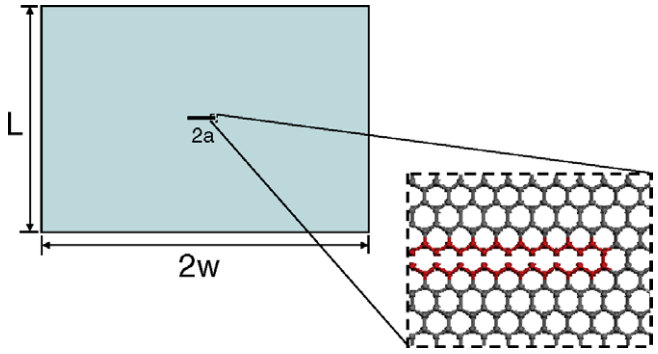

Fig. 1. The dimension of the graphene sheet with center crack where L = 1022.4 Å, $2w$ = 1475.8 Å and $2a$ = 100.8 Å.

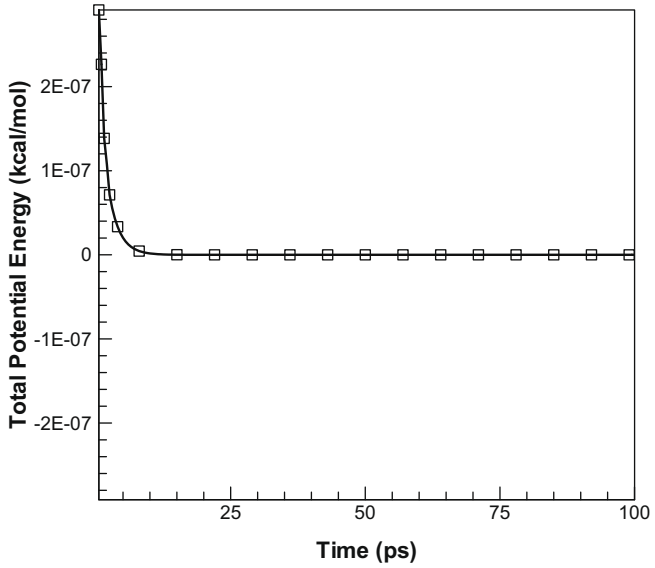

Fig. 2. Total potential energy histories during the NPT ensemble in MD simulation.

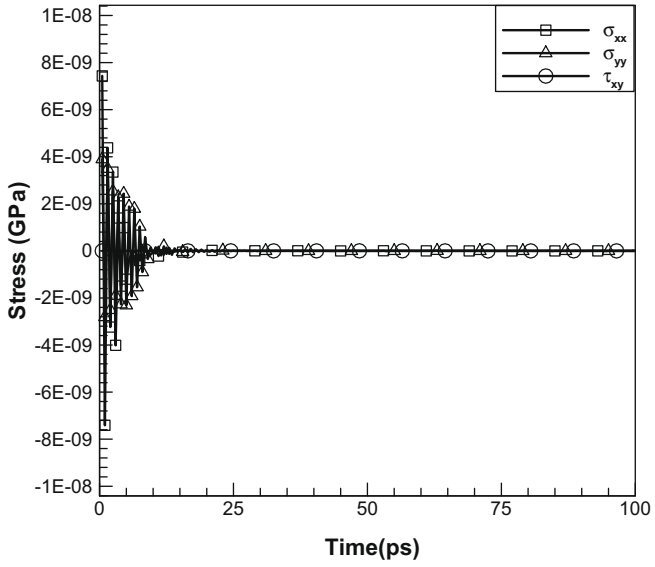

Fig. 3. Stress histories during the NPT ensemble in MD simulation.

of stress intensity factor can be defined accordingly and utilized to characterize the fracture behavior. Based on the linear elastic fracture mechanics concept, we attempted to measure the local stress field in the discrete atomistic model and to understand if there is singular stress field existing in the vicinity of the crack tip. There have been various definitions of local stress in atomistic simulation such as virial stress, BDT (atomic) stress (Basinski et al., 1971), Lutsko stress (Cormier et al., 2001), and Hardy stress (Hardy, 1982). Numerical results demonstrated that the Hardy is appropriate for both homogeneous and inhomogeneous deformation; moreover, it is very accurate and robust, and it is superior to BDT and Lutsko stress formulation in the local stress calculation (Zimmerman et al., 2004; Webb et al., 2008). Thus, the Hardy stress formulation expressed as

$$\boldsymbol{\sigma}(\mathbf{r},t)=\left\{\sum_{\alpha=1}^{N} m^{\alpha}(\mathbf{v}^{\alpha}-\mathbf{v})\otimes(\mathbf{v}^{\alpha}-\mathbf{v})\psi(\mathbf{r}^{\alpha}-\mathbf{r})+\frac{1}{2}\sum_{\alpha=1}^{N}\sum_{\beta\neq\alpha}^{N}\mathbf{r}^{\alpha\beta}\otimes\mathbf{F}^{\alpha\beta}B^{\alpha\beta}(\mathbf{r})\right\} \tag{4}$$

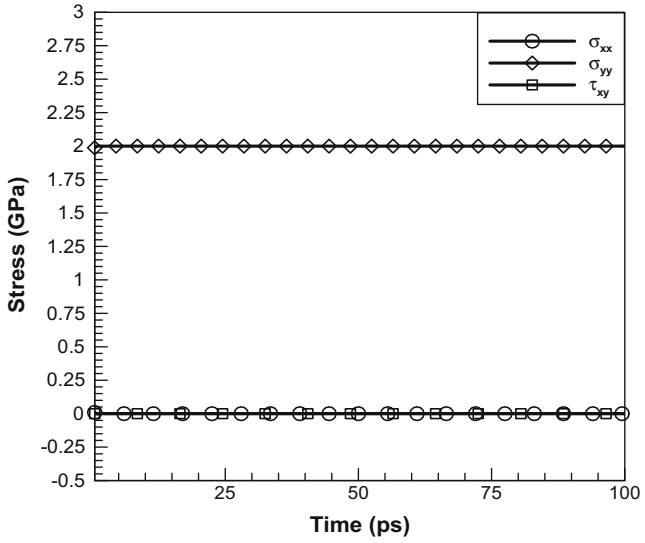

Fig. 4. Stress histories in the modified NPT ensemble with $\sigma_{yy}=2GPa$.

was employed to evaluate the local stress field near the crack tip of the graphene sheet, where m^{α}, $\mathbf{v}^{\alpha}$ and $\mathbf{r}^{\alpha}$ represent the mass, velocity and position of atom α, respectively; $\mathbf{v}$ and ψ represent the continuum velocity and localization function. In addition, $\mathbf{r}^{\alpha\beta}=\mathbf{r}^{\alpha}-\mathbf{r}^{\beta}$ and $\mathbf{r}^{\alpha}$ and $\mathbf{r}^{\beta}$ represent the position of atom α and β, respectively. $\mathbf{F}^{\alpha\beta}$ is the force between atoms α and β. By considering the localization function ψ as a Gaussian function

$$\psi(\mathbf{r}^{\alpha}-\mathbf{r})=\frac{1}{(\sqrt{\pi}h)^{3}}\exp\left[-\frac{(\mathbf{r}^{\alpha}-\mathbf{r})^{2}}{h^{2}}\right] \tag{5}$$

bond function $B^{\alpha\beta}(\mathbf{r})$ is then expressed as

$$B^{\alpha\beta}(\mathbf{r})=\int_{0}^{1}\frac{1}{(\sqrt{\pi}h)^{3}}\exp\left[-\frac{(\lambda\mathbf{r}^{\alpha\beta}+\mathbf{r}^{\alpha}-\mathbf{r})^{2}}{h^{2}}\right]d\lambda \tag{6}$$

where h is the smoothing length and is equal to 1.9 at the present simulation. It is noted that the kinetic term in Eq. (4) would equal zero when the analysis is performed at zero temperature. In addition, the size of the localization volume used in the stress calculation is 10 Å. During the employment of Hardy formulation, the angle bond interaction given in Eq. (3) needs to be converted into the atomic forces acting on the atoms, the detail procedure can be found elsewhere (Machida, 1999).

2.3. Calculation of strain energy release rate

In addition to the stress intensity factor, the strain energy release rate is the other fracture parameter that has been frequently used in the linear elastic fracture mechanics. In order to apply the concept of the strain energy release rate in the discrete atomistic model, the energy difference before and after the crack extension has to be calculated appropriately. Two methods, global energy method and crack closure method, are introduced to determine the energy difference.

2.3.1. Global energy method

In the atomistic simulation, the total energy is contributed from the potential energy because of the bonded interaction and the kinetic energy caused by the atomistic thermal oscillation. Because the simulation is conducted at 0 K, the effect of kinetic energy can be neglected, and the potential energy is regarded as the total energy of the discrete graphene system. When the atomistic configuration of the cracked graphene sheet under remote loading

was obtained through MD simulation, the potential energy of the system with crack length equal to $2a$ was calculated based on the bonded potential function given in Eqs. (2) and (3). Subsequently, the center crack length was extended from $2a$ to $2a + 2\Delta a$ by removing the covalent bonds in the crack tips. Because of the characteristics of the discrete structure, the crack extension length Δa is equal to the lattice size of graphene, 2.45 Å. Berendsen NVT ensemble (Berendsen et al., 1984) was carried out on the new system (crack length equal to$2a + 2\Delta a$) for 100 ps to achieve the total energy minimization; meanwhile, the minimized value of the total energy was directly calculated from the MD simulation. It is noted in the NVT ensemble that the whole volume of the system is remaining fixed, and no external work was supplied into the system. As a result, the total energy variation being considered as the energy loss during the crack extension can be utilized to calculate the strain energy release rate of the atomistic graphene structures as follows:

$$G = -\frac{U_{2a+2\Delta a} - U_{2a}}{2\Delta a t} \tag{7}$$

where $U_{2a+2\Delta a}$ is the potential energy of the graphene sheet with crack length $2a + 2\Delta a$, and U_{2a} is the potential energy of the graphene sheet with crack length $2a$. In addition, "t" is the thickness of the graphene that is assumed to be 3.4 Å (Iijima et al., 1992).

2.3.2. Crack closure method

The energy difference during the crack extension in the atomistic structure can also be calculated from the crack closure concept where the amount of energy variation during the crack extension is equal to the work required to close the crack back to its original length ($2a$). This concept, originally proposed by Irwin (1957), was normally adopted to measure the strain energy release rate in continuum media. The work needed to close the crack for a Mode I fracture can be estimated as

$$\Delta W = \frac{1}{2}\sum_{i=1}^{3} F_{iy}(u_{iy}^{+} + u_{iy}^{-}) \tag{8}$$

where F_{iy} is the concentrated force acting on atoms A_i and B_i when crack length is $2a$, and u_{iy}^{+} and u_{iy}^{-} are the corresponding opening displacement for the atoms A_i and B_i as shown in Fig. 5 when the crack extends $2\Delta a$. In the MD simulation, the force F_{iy} is obtained by artificially removing the corresponding covalent bonds (one stretching bond and four angle bonds) and then calculating the unbalanced forces acting on atoms A_i and B_i. It is noted that the unbalanced forces are only present on the atoms A_i and B_i. ($i = 1$–3) when the corresponding covalent bonds (one stretching bond and four angle bonds) are eradicated from the graphene structure, and thus the work required to close the crack can be evaluated in terms of the unbalanced forces and the corresponding displacement of the atoms. Because of symmetric geometry and loading conditions, the calculated unbalanced forces are almost the same, but they are acting in the opposite directions as illustrated in Fig. 5. Moreover, the displacement of atoms A_i and B_i after the crack extension can be simply obtained by measuring the corresponding position vectors in the MD simulation. It is noted that in the continuum media, the work estimated from Eq. (8) can be directly used in the calculation of stain energy release rate. However, for the discrete atomistic system, in addition to the work done, the bonded energy that was eradicated during the crack extension has to be recovered in order for the discrete system to be completely back to its original state. In other words, the covalently bonded energy contributed from the stretching bond and the angle bending bond has to be evaluated and accounted for in the crack closure method. In each crack tip, the potential energy needed to be retrieved contains one stretching bond (bond a) and four angle bending bonds

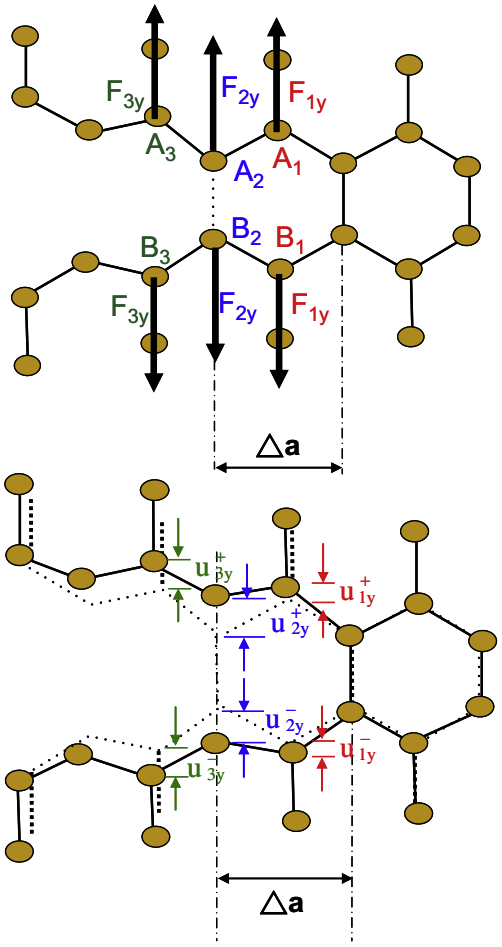

Fig. 5. Atomic force and opening displacement in Mode I fracture for graphene sheet.

(bonds b, c, d and e) as shown in Fig. 6. Table 1 illustrates the potential energy associated with these interatomistic bonds. Thus, the recaptured potential energy in each crack tip can be written as

$$E_{\text{bonds}} = (E_a + E_b + E_c + E_d + E_e) \tag{9}$$

A combination of Eqs. (8) and (9) yields the total energy release associated with the crack extension of Δa, from which the Mode I strain energy release rate for the graphene sheet is deduced as

$$G_I = \frac{1}{2\Delta a t}(2\Delta W + 2E_{\text{bonds}}) \tag{10}$$

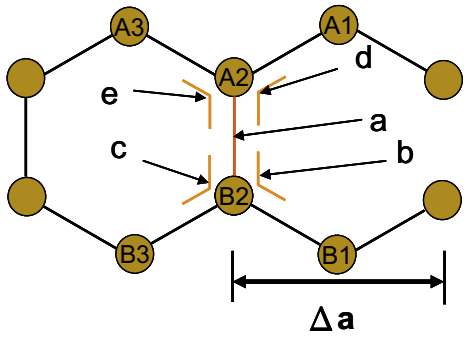

Fig. 6. The bonded energy should be recovered in crack closure method for the atomistic graphene structure.

Table 1
Bonded energy for discrete graphite structure under mode I loading.

Stretch bond (a)	Angle bond (b) (d)	Angle bond (c) (e)
0.111	0.029	0.000027

Unit: kcal/mol.

In the same manner, the work needed to close the crack for Mode II fracture can be estimated as

$$\Delta W = \frac{1}{2}\sum_{i=1}^{3} F_{ix}(u_{ix}^{+} + u_{ix}^{-}) \tag{11}$$

where F_{ix} is a concentrated force acting on atoms A_i and B_i in the x direction. In addition, u_{ix}^{+} and u_{ix}^{-} are the sliding displacement for the atoms A_i and B_i, respectively, when the crack extend in sliding mode. Again, the strain energy release rate for the Mode II fracture in the atomistic graphite sheet can be expressed in terms of the crack closure method as

$$G_{\mathrm{II}} = \frac{1}{2\Delta a t}(2\Delta W + 2E_{\mathrm{bonds}}) \tag{12}$$

where E_{Bonds} denotes the potential energy should be recovered from the covalent bonds associated with the shear deformation of the graphite sheet.

3. Continuum model

In the previous section, the graphene was modeled as a discrete atomistic structure, and the energy difference during crack extension was calculated from the MD simulation. On the other hand, when the graphene sheet was characterized as an isotropic homogeneous solid, the fracture parameters, i.e., stress intensity factor and strain energy release rate, can be determined simply from the LEFM. It is noted that in the continuum model, the atomically blunt crack was assumed to be a line sharp crack in the LEFM analysis. It is an interesting task to determine if the fracture parameters calculated from the LEFM would be compatible to those obtained from the atomistic graphene sheet model. To understand if there is a fracture parameter being able to bridge the gaps between the discrete and continuum models would be the main concern of the study. In order to resolve the aforementioned questions, the fracture parameters of the continuum model, i.e., strain energy release rate as well as the stress intensity factor, were calculated based on LEFM theory, and the results were compared to the corresponding atomistic simulation.

Table 2
Material properties of graphene sheet obtained from MD simulation.

Young's modulus (GPa)	Shear modulus (GPa)	Poisson's ratio
790.7	311	0.27

For a finite plate with a center crack, the stress intensity factor can be approximated in a polynomial form as (Anderson, 1995)

$$K = \sigma\sqrt{\pi a}\left[\sec\left(\frac{\pi a}{2W}\right)\right]^{1/2}\left[1 - 0.025\left(\frac{a}{W}\right)^2 + 0.06\left(\frac{a}{W}\right)^4\right] \tag{13}$$

where a is the half crack length, W is the half graphene width, and σ is the remote loading acting on the graphite sheet. Because the graphene sheet is pretty thin, the plane stress condition was assumed in the modeling, and thus the strain energy release rate can be expressed in terms of stress intensity factor as

$$G = \frac{K^2}{E} \tag{14}$$

where E is the Young's modulus of the graphene sheet. It is noted that the material properties utilized in the continuum model was calculated based on the molecular dynamics simulation with the interatomistic energy described earlier, and the results are presented in Table 2.

In addition to the analytical LEFM solution, the finite element method is an alternative technique to evaluate the fracture parameters in continuum solids. Fig. 7 illustrates the mesh of the graphene sheet. It is noted that the fine meshes in the vicinity of crack tips were generated in order to precisely simulate the singular stress field. For the comparison purpose, the same geometric configuration and loading condition as used in the atomistic simulation was introduced in the FEM model. The stress intensity factor of the continuum solid can be determined from the near-tip stress field (Sanford, 2003) as

$$K_{\mathrm{I}} = \lim_{r\to 0}\sigma_{yy}\sqrt{2\pi r} \tag{15}$$

$$K_{\mathrm{II}} = \lim_{r\to 0}\sigma_{xy}\sqrt{2\pi r} \tag{16}$$

where K_{I} and K_{II} are Mode I and Mode II stress intensity factor, respectively, and σ_{yy} and σ_{xy} are the tensile and shear stress components near the crack tip. In addition to the stress intensity factor, the strain energy release rate of the continuum graphene sheet can be determined from the finite element method using the crack closure integral (Sun and Jih, 1987) as

$$G_{\mathrm{I}} = \lim_{\delta a\to 0}\frac{1}{2\delta a} f_y^b(u_y^a - u_y^{a\prime}) \tag{17}$$

$$G_{\mathrm{II}} = \lim_{\delta a\to 0}\frac{1}{2\delta a} f_x^b(u_x^a - u_x^{a\prime}) \tag{18}$$

where f_x^b and f_y^b denotes the nodal force at node b in the x and y direction. u_x^a and u_y^a are the displacement components at node a, and $u_x^{a\prime}$ and $u_y^{a\prime}$ are the displacement components at node a' as shown in Fig. 8.

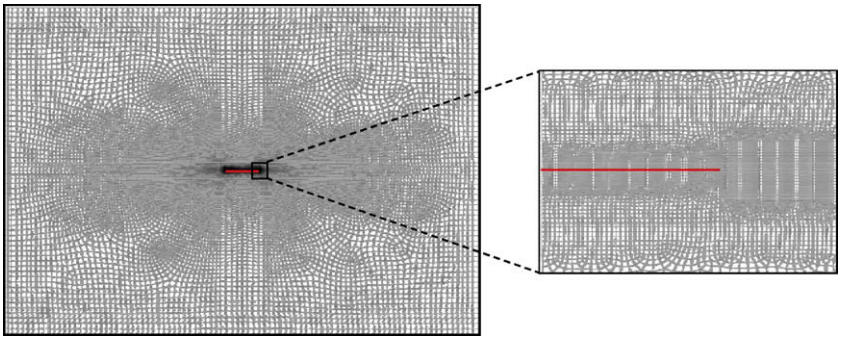

Fig. 7. The finite element meshes for the continuum graphene model.

4. Results and discussion

Fig. 9 illustrates the stress distribution near the crack tip obtained from the continuum model (FEM solution and LEFM solution) as well as the atomistic model associated with the same remote tensile loading. Apparently, the stress field calculated based on the LEFM solution and the FEM solution demonstrates $1/\sqrt{x}$ stress singularity near the crack tip. On a contrary, in the discrete atomistic model, the stress field begins to deviate from the $1/\sqrt{x}$ singularity solution in one lattice distance from the crack tip; therefore, there is no apparent stress singularity observed near the crack tip. This non-singular stress field in the atomistic model could be attributed to two possible reasons. One reason is that near to the crack tip where the deformation gradient is high, the expression of Hardy stress is expected to be non-local (Eringen et al., 1977). The other one could be the atomically blunt crack tip in the atomistic model, which may be responsible for the non-singular stress. No matter which one caused the non-singular stress field, it is evident that adopting the stress intensity factor concept in the atomistic model may make the fracture parameter ambiguous. In addition, it was found that when the position is beyond one lattice spacing from the crack tip, the stress field calculated from the discrete model coincides with the FEM solution well. The same attributes of the stress field was also observed in the Mode II fracture when the graphene sheet is subjected to remote shear loading. Because of the characteristic of the non-singular stress at the crack tip, it is suggested that the stress intensity factor defined based on singular stress assumption may not be suitable for describing the fracture in the discrete model.

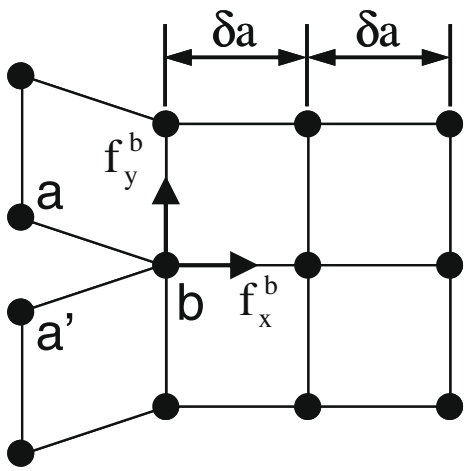

Fig. 8. Schematic of crack closure technique used in FEM analysis.

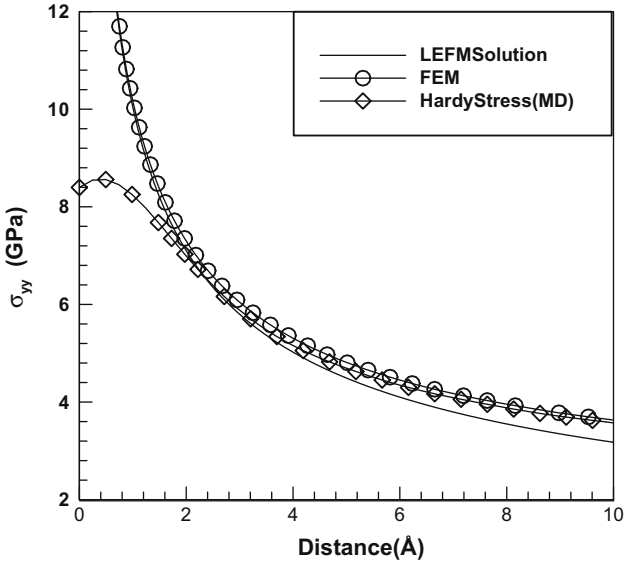

Fig. 9. Stress distribution near the crack tip obtained from the continuum model (FEM solution and LEFM solution) and atomistic model.

The calculation of total energy variations obtained from the global energy method and crack closure method for Mode I crack extension in molecular dynamics simulation are illustrated in Table 3. Moreover, the strain energy release rates for the Mode I fracture calculated based on the discrete atomistic model and its continuum counterpart are presented in Table 4. It can be seen that the strain energy release rates obtained from the continuum model is in good agreement with those in discrete model. Moreover, both the global energy method and the crack closure method provide almost the same strain energy release rate in the discrete graphene model. Since the global energy method in the MD simulation is relatively simple, it was suggested that it be utilized in the calculation of the strain energy release rate in the molecular simulation. Similar tendency for the Mode II fracture of graphene sheet was also observed, and the corresponding results are presented in Tables 5

Table 3
Comparison of total energy variation calculated based on global energy method and crack closure method during crack extension in MD simulation (Mode I case).

Global energy method	Crack closure method	
Total energy variation	ΔW	E_{bonds}
1.95	1.61	0.34

Unit: kcal/mol.

Table 4
Comparison of strain energy release rate obtained from continuum model and discrete atomistic model (Mode I case).

	Continuum model		Atomistic model	
	LEFM (finite plate)	FEM	Global energy method	Crack closure method
Strain energy release rate (J/m^2)	0.081	0.0794	0.0814	0.0809

Table 5
Comparison of total energy variation calculated based on global energy method and crack closure method during crack extension in MD simulation (Mode II case).

Global energy method	Crack closure method	
Change in total potential energy	ΔW	E_{bonds}
0.504	0.351	0.151

Unit: kcal/mol.

Table 6
Comparison of strain energy release rate obtained from continuum model and discrete atomistic model (Mode II case).

	Continuum model		Atomistic model	
	LEFM (finite plate)	FEM	Global energy method	Crack closure method
Strain energy release rate (J/m^2)	0.0201	0.0203	0.021	0.0208

and 6. In light of the forgoing, it is revealed that the strain energy release rate can be regarded as a physical quantity that is capable of establishing connections between the atomistic simulation and the continuum media for characterizing the fracture of covalently bonded graphene sheet.

5. Conclusion

The fracture behavior of a graphene sheet with a center crack was characterized using atomistic simulation and linear elastic fracture mechanics (LEFM). In the atomistic simulation, the graphene was regarded as an atomistic structure, containing discrete carbon atoms; nevertheless, in the LEFM, it was modeled as an isotropic homogeneous media. Results from atomistic simulation indicated that because of the discrete attribute, there is no stress singularity near the crack tip. Therefore, the concept of stress intensity factor, which is generally employed in the continuum mechanics, may not be suitable for modeling the crack behavior in the atomistic graphene sheet. In order to validate the strain energy release rate concept, the energy variation before and after the crack extension were evaluated in both continuum and atomistic model. For the discrete atomistic model, two methods, i.e., the global energy method and the crack closure method, were employed to compute the energy variation as well as the strain energy release rate. On the other hand, the finite element analysis was performed in the continuum graphene sheet for the estimation of the strain energy release rate. It was denoted that the strain energy release rate calculated based on the global energy method and crack closure method are almost the same. Furthermore, it was demonstrated that the global energy method is a simple manner in the atomistic simulation for the calculation of the strain energy release rate. A comparison of atomistic simulation with finite element results illustrated that the strain energy release rates obtained from continuum model coincided with that in the discrete model associated with the same loading condition. As a result, the concept of strain energy release rate is regarded as a physical quantity that can establish connections between the atomistic simulation and continuum modeling for modeling the fracture of covalently bonded graphene sheet.

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