Tensile Deformation and Fracture Mode of Graphene Irradiated by Carbon Atoms

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***Abstract* — Irradiation is an important way to cut and modify graphene in engineering. But in the process of irradiation, different kinds of defects may be produced, which may affect the properties of graphene, such as the tensile deformation and fracture mode. So, to investigate the defect influence on tensile deformation and fracture mode of graphene, the present paper established the numerical model of graphene irradiated by Carbon Atoms (C), as well as the tensile model of irradiated graphene by using molecular dynamics (MD) method. Based on simulation results, tensile deformation and fracture mode of irradiated graphene were investigated. Compared with the perfect graphene, the results indicate that the tensile deformation and fracture mode of irradiated graphene is essential different from that of perfect graphene.**

Keywords - Graphene;Irradiation;Tensile deformation;Fracture mode

I. INTRODUCTION

Graphene is a new type of high performance nano-material. Irradiation is an important way to cut and modify graphene in engineering. But in the process of irradiation, because of randomness of incident particles, irradiated defects will be inevitably produced [1], which may seriously affect the mechanical properties of graphene.

Recently, many researches on irradiated graphene have been implemented. Giuseppe Compagnini [3] analyzed the formation process of irradiated defects of single-layer graphene, and compared performances of irradiated grapphene with perfect graphene. L.Tapaszto [4] investigated ion irradiation influence on graphene electronic structure, and results indicated that irradiation could change the electronic hybrid mode. Marks [5] set up the relationship between incident ions and steady-state stress. Sachin S.Terdalkar [6] studied ion irradiation effects on deformation of graphene by MD method. O Lehitinen [7] set up the kinetic monte-carlo method to study morphology changes in the process of irradiation by using MD method, and the influences of incident angles, incident ions and energy on graphene was also studied. Xin Wu [8] solved the connection problems between graphene layers by using ion irradiation, and realized production of large area graphene, which had a very important role for the application of graphene.

In the present paper, by using MD method, the numerical model of graphene irradiated by C Atoms, as well as the tensile model of irradiated graphene were established. In addition, compared with the perfect graphene, tensile deformation and fracture mode of graphene irradiated by C Atoms was investigated.

II. MODELING AND COMPUTATIONAL DETAILS

A. Irradiation Model

By using MD simulation software LAMMPS, the present paper establishes the numerical model of graphene irradiated by C Atoms. The size of model is 8.30×8.36nm, which includes 2760 carbon atoms. Atomic configuration diagram of the model is shown in Fig. (1).

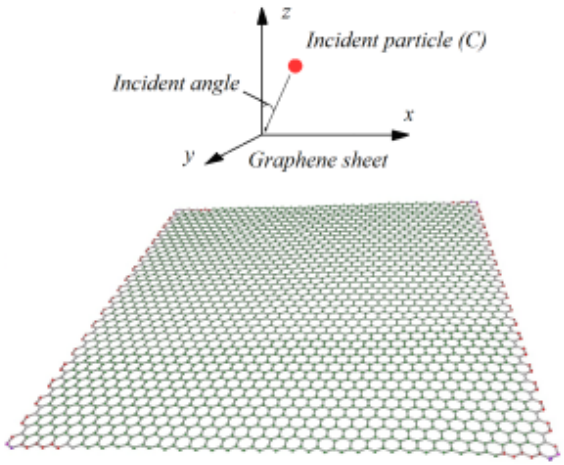

Fig.1. Atomic Configuration Diagram of The Model Irradiated By C Atoms

According to Fig.1, the initial position of incident C Atoms locate above a certain height of graphene sheet, and then irradiate graphene sheet at a certain angle and speed.

In the model, AI-REBO potential function is used to describe the interactions between graphene atoms, while

Tersoff/ZBL potential function is used to describe the interactions between the incident C atoms and graphene atoms. Tersoff/ZBL potential function is formed by joining the Tersoff [9] potential function and Ziegler-Biersack-Littmark（ZBL) [10] potential function together smoothly, which is a good description of the collision process of irradiation. The total energy of Tersoff/ZBL potential is expressed by the following equation:

$$E = \frac{1}{2}\sum_{i}\sum_{j\neq i} V_{ij} \tag{1}$$

in which, the bond energy V_{ij} is written as:

$$V_{ij} = (1 - f_F(r_{ij}))V_{ij}^{ZBL} + f_F(r_{ij})V_{ij}^{Tersoff} \tag{2}$$

where $f_F(r_{ij})$ is the function that make sure the ZBL potential function connect smoothly with the Tersoff potential, which can be written as:

$$f_F(r_{ij}) = \frac{1}{1+e^{-A_F(r_{ij}-r_C)}} \tag{3}$$

In addition, the ZBL potential is as follows:

$$V_{ij}^{ZBL} = \frac{1}{4\pi\varepsilon_0}\frac{Z_1 Z_2 e^2}{r_{ij}}\phi(r_{ij}/a) \tag{4}$$

In which, r_C is the cutoff distance; Z_1 and Z_2 are proton numbers; e is electronic charge; ε_0 is dielectric constant; r_{ij} is the distance between atom i and atom j. And the constant a is as follows:

$$a = \frac{0.8854a_0}{Z_1^{0.23} + Z_2^{0.23}} \tag{5}$$

The function $\phi(x)$ is:

$$\begin{aligned}\varphi(x) = {} & 0.1818e^{-3.2x} + 0.5099e^{-0.9423x} \\ & + 0.2802e^{-0.4029x} + 0.02817e^{-0.2016x}\end{aligned} \tag{6}$$

In the tensile model, Tersoff potential is used, whose total energy can be written as:

$$E = \sum_i E_i = \frac{1}{2}\sum_{i\neq j} V_{ij} \tag{7}$$

in which

$$V_{ij} = f_c(r_{ij})[f_R(r_{ij}) + b_{ij} f_A(r_{ij})] \tag{8}$$

where V_{ij} is the bond energy of atom i and j, while f_A is bond order function; f_R is attraction and repulsion of pair potential.

These potentials choice is supported by previous simulation results, which showed good coincident with experimental data.

Atomic mass of C is set as 12.01, and time step is 1*fs*. In *x* and *y* directions, non-periodic and shrink-wrapped boundary conditions *s* are applied. And the Nose-Hoover isothermal adjustment method is used.

Firstly, the tensile model is fully relaxed until it reaches the equilibrium state. And then, the upper and lower ends of a layer of carbon ring are fixed. In the NVT ensemble, the model is uniformly stretched with a strain rate of 10-9 s^{-1}. After each stretch, the model is relaxed for 1*ps* until the graphene is fracture.

Firstly, model is fully relaxed until it reaches the equilibrium state. And then, three layers of atoms are fixed at both sides of graphene. In *x* and *y* directions, non-periodic and shrink-wrapped boundary conditions *s* are applied, while non-periodic and shrink-wrapped with a minimum value boundary condition *m* is applied in *z* direction.

In the process of irradiation, the initial positions of incident C atoms with different energy distribute randomly just above the graphene sheet, and then irradiate the graphene sheet one by one. After each incidence, the graphene sheet is relaxed for 1*ps* until the temperature return to the initial temperature 300K.

B. Tensile Model

To investigate the tensile deformation and fracture mode of irradiated graphene, the tensile model of graphene irradiated by C atoms is established, as shown in Fig.2.

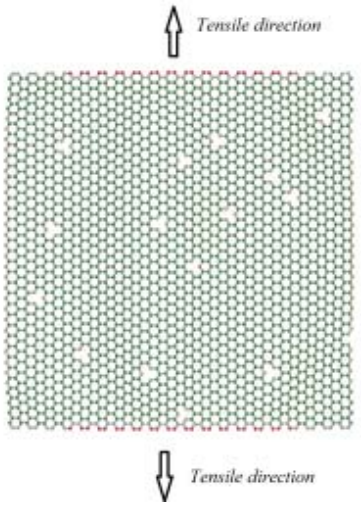

Fig.2. Atomic Configuration Diagram of Tensile Model Irradiated By C Atoms

III. RESULTS AND DISCUSSIONS

A. Defects Extension

In the present paper, graphene irradiated by 30 and 70 incident C atoms are investigated which is shown in Fig.3(a) and (b). According to the irradiated results, there are many

kinds of irradiated defects in the graphene model, such as single vacancy defect, double vacancy defect and so on.

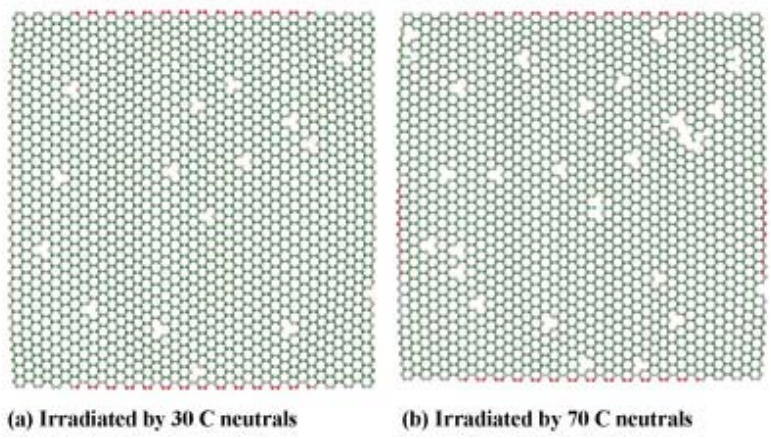

Fig.3. Atomic configuration diagram of gaphene irradiated by 30 and 70 C Atoms

Fig.4(a) and (b) are the tensile atomic configuration diagram . According to the Fig.4, defects at the graphene edges will firstly begin to extend, as shown in red circle. It is because the number of atomic bonds at the edge is less than that inside of graphene, so it leads to the lower lattice bonding energy at the edge. In addition, the existence of defects at the edge further weakened the lattice bond energy. So vacancy defects at the edge firstly begin to extend, just as that in the Fig.4.

After that, vacancy defects inside the graphene begin to propagate one after another, which is shown in Fig.5. Most of single vacancy defects extend and form new types of defect like double vacancy defect as shown in red square and other more complicated defect as shown in red rhombus . But there are also several single vacancy defects have not extended yet.

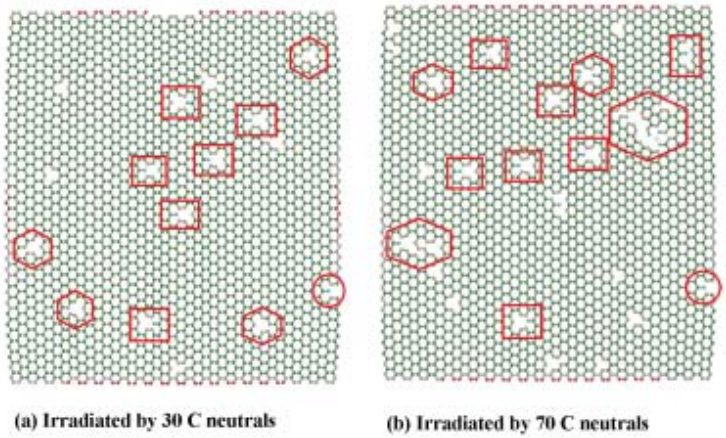

Fig.4. Atomic configuration diagram of extension of defects at the edge

B. Formation of Defect Clusters

And then, defects will further propagate, and the influence area of defect increases gradually. The adjacent defect regions interconnect and form defect clusters, as shown in Fig.5. With the continuous increase of tensile load, clusters of defects will further propagate and form defect area perpendicular to the tensile direction, as shown in Fig.6, which form weak fracture belt of graphene.

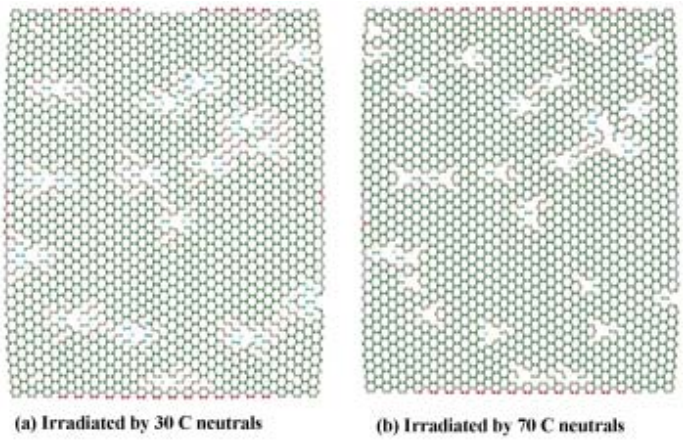

Fig.5. Adjacent defect regions interconnect and form defect clusters

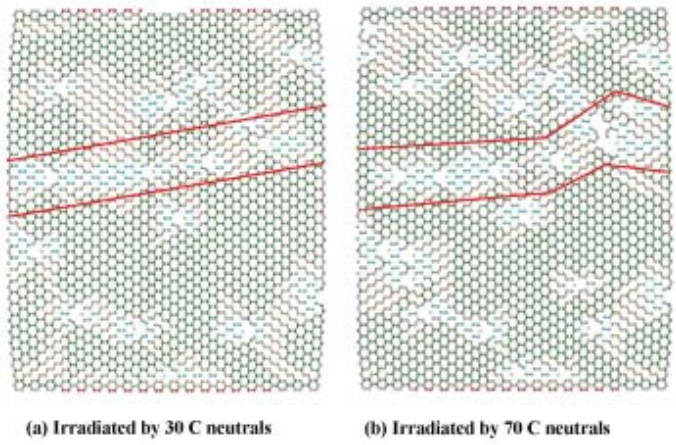

Fig.6. Defect area perpendicular to the tensile direction

C. Formation of Weak Zone and Fracture

When it comes to the fracture mode of irradiated graphene, there are two situations. One is that the fracture begins at the edge of graphene as shown in Fig.7(a), which propagates along the diagonal lines to the other side of graphene, as shown in Fig.8(a). For this situation, defect types of graphene is almost single vacancy, so failure mode is almost the same as that of perfect graphene.

For another fracture mode, the fracture begins inside of graphene as shown in Fig.7(b), and propagates to both external edges of graphene, as shown in Fig.8(b). For this situation, the point at which the fracture begin to propagate just the place where the multi vacancy defect locates, so this kind of failure mode is different from that of perfect graphene.

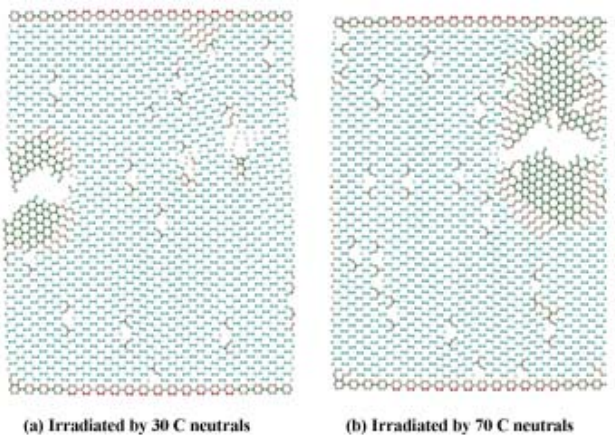

Fig.7. Fracture mode of irradiated graphene

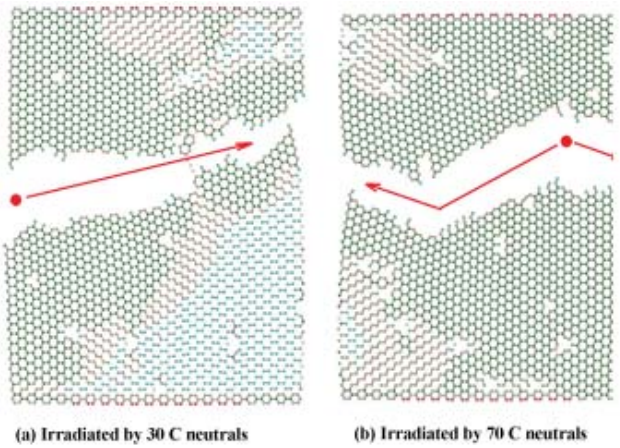

Fig.8. Fracture propagation（dot represents the fracture starting point, arrow represents fracture direction）

D. Analysis of Tensile Deformation and Fracture Mode

According to literatures [2] and [11], for perfect graphene, tensile fracture began at one side of graphene, and then propagated along 45° direction of graphene until graphene was completely broken.

Compared with perfect graphene, tensile deformation and fracture mode of graphene irradiated by C atoms include three stages, namely the single defect propagation, defect cluster formation, weak zone formation and fracture. The fracture mode of irradiated graphene depends mainly on the type of defect and location. That is to say, if defects are all single vacancy defect, then the fracture is almost the same as that of perfect graphene. On the other hand, if there are multi-vacancy defects, then the fracture begins at the place where the multi vacancy defect locates, and propagates to both external edges of graphene.

IV. CONCLUSIONS

Based on the results above, several conclusions are obtained as follows,

(1) Compared with perfect graphene, tensile deformation and fracture mode of graphene irradiated by C atoms include four stages, namely the single defect extension, defect cluster formation, weak zone formation and fracture.

(2) The fracture mode of irradiated graphene depends mainly on the type of defects and their location.

(3) If defects are all single vacancy defect, then the fracture is almost the same as that of perfect graphene. In the other hand, if there are multi-vacancy defects, then the fracture begins internal at the place where the multi-vacancy defect locates, and extends to both external edges of graphene.

CONFLICT OF INTEREST

The authors confirm that this article content has no conflicts of interest.

ACKNOWLEDGMENT

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