# Structure Evolution and Nature of Defects in Bcc Iron by Collision Cascade from Molecular Dynamics Simulation

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**Abstract:**

The structure evolution and nature of defects in bcc iron by collision cascade from molecular dynamics simulation are investigated. Under irradiation, the collision cascade induces not only self-interstitials, vacancies, <100>, <110>, and <111> dumbbell defects, but also, composite defects, such as, the composite defect of <110> and <111> dumbbell, and composite defect of <110>, <110> dumbbell, and defect clusters. Simulation shows that under the considered energy of primary knock-on atom the higher the energy of a primary knock-on atom (PKA) is, the more the number of producing interstitials is. The size of the region where atoms are displaced by the collision cascade is about 11-15$a_0$. The smaller the energy of PKA is, the smaller the region is. At the same time, it is found that even at the initial stage of 0.0-0.75 ps of collision cascade, there is also some recombination of interstitials and vacancies.

Key words: Molecular Dynamics; Displacement collision cascade , cascade damage

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## I. Introduction:

In a future fusion nuclear power plant, the structural materials used in fusion reactors are exposed to neutron fluences with irradiation doses of about 1-10$\times 10^{23}$nm$^{-2}$ over a 40-60 year

service life. These materials will undergo severe embrittlement under the neutron irradiation. This effect is attributed to the microstructure evolution of defects under irradiation, because the microstructure evolution leads to matrix damage accumulation and grain boundaries segregation. However, the properties of the defects and the detail about the evolution process are peculiar and their physics is not yet completely understood [1]. As well known, under irradiation the interaction between impinging particles and materials may last a few of femtosecond in matrix materials, and lead to the acceleration of the so-called primary knock-on atom (PKA). The accelerated PKA starts the development of a cascade of atomic displacements, and induces a large amount of defects. Ultimately, these defects may be developed into dislocation loops, stacking fault, and cavities such as void and He bubbles[2]. They will lead to a change in the mechanical properties of materials, such as hardening, embrittlement, loss of ductility and fracture toughness. Although the spatial and temporal resolutions required to investigate a cascade evolution are not available by any experimental methods, the use of molecular dynamics (MD) simulations makes it possible to study such a cascade process with spatial size at atomic scale and temporal resolution at femtosecond level.

MD simulations have such a capacity to provide a picture of the evolution and formation of displacement cascade in detail. For example, Yu et al simulate the cascade collision of He in Fe and find that the interstitial dumbbell of Fe–Fe and Fe–He are in the <1 0 0> and <1 1 0> lattice direction[3]. Kwon, Kim, and Hong compare the primary damage states iron and nickel by MD simulation [4]. They find that the bcc-Fe displacement cascade produced more residual defects than the fcc-Ni cascade. In addition, they also observe various sizes of interstitial clusters in Ni. Using molecular dynamics simulation Stoller study the effect of PKA energy on point defects [4].

They find that although the amount of point defects produced is not linearly proportional to the PKA energy, a higher energy PKA tends to produce more defects in the displacement cascade. A lower energy PKA is more efficient at point defect production than a higher energy PKA, whereas a higher energy PKA produce more defect cluster that can make a contribution to the formation of extended defects [4]. Two primary stable interstitial configurations of <110> and <111> dumbbells are also observed in bcc iron by Stoller et al [5]. Simulation of cascades in iron by MD based on many-body potential shows that the cluster configurations of self-interstitial atoms (SIA) are made of nonparallel dumbbells form spontaneously [6]. More recent MD studies confirm the formation of SIA clusters in nonparallel configurations, not only in cascades [7], but also during cluster migration at high temperature [7]. By MD simulation Terentyev et al also find small interstitial-type defects in bcc iron with complex structures and very low mobilities [1]. Satoh, Matsui, and Hamaoka reveal a physical picture of one-dimensional migration of interstitial clusters in bcc iron by MD simulation [8]. However, the recombination of interstitials and vacancies at the initial stage of collision cascade and the size of collision cascade region are not reported in the above works. In this work, the cascade of PKA in bcc iron at two different PKA energies at the temperature of 500K is further investigated by MD simulation, and the nature of defect evolution at two energies of PKA is further presented. A kind of composite defects is found. Under the considered energy of PKA the size of the region where atoms are displaced by the collision cascade is about 11-15$a_0$, $a_0$ is lattice constant. The smaller the energy of PKA is, the smaller the region size is. At the same time, it is also found that even at the initial stage of 0.0-0.75 ps of collision cascade, there is also some recombination of interstitials and vacancies.

**II Simulation method and procedure**

In the present work, the interatomic potential for Fe-Fe interaction is described based on embedded atom method and parameterized by Ackland, Mendelev, Srolovitz, et al [9]. For the extreme short range repulsion, which is used in a cascade simulation, the screened electrostatic form of Biersack and Ziegler is adopted [10]. Between the range used for the universal screening function and that employed for the embedded atom method, a simple interpolation scheme is used, with coefficients chosen to ensure that the pair function and its first derivative are continuous at its two end points connecting with the embedded atom method and the screening function. This potential has been used to describe the properties of defects in bcc iron very well [9].

A molecular dynamics code [11], which has been modified to simulate nano-frication[12], is now used to be appropriate for a collision cascade simulation for a bcc Fe. The computational cell includes 16000 Fe atoms in a bcc structure initially. The periodic boundaries are applied along the X[100], Y[010], and Z[001] direction of the cell. The atomic motion under constant temperature condition is realized by using an improved Verlet algorithm [13] to integrate Hoover equation [14]. The equation has a form as follows:

$$m_i \ddot{r}_i = F_i + \left(\sum_{j(\neq i)} F_j \cdot \dot{r}_j \Big/ \sum_{j(\neq i)} (m_j \cdot r_j^2)\right) \cdot m r_i, \qquad i = 1,2,3,...,n \tag{1}$$

In the above equation, $m_i$ and $\ddot{r}_i$ are the mass and acceleration of atom *i*, respectively. The force $F_i$ is the derivative of total potential with respect to the atom coordinates $r_i$, and it is now a function of both atom positions and atom electron densities. While the constraint force (the second term of the right side in the equation (1)), which constrains the kinetic energy of the system, is

now a function of atom positions, atom velocities $\dot{r}_i$ and electron densities. Thus, by using an embedded atom method potential to perform MD simulation, the contribution from electrons is taken into account.

In order to simulate a collision cascade in bcc Fe, the cascade simulations are initiated by giving the primary knock-on Fe atom the appropriate amount of kinetic energy. Here index direction of <1 1 0> is chosen as the direction of PKA kinetic energy. This special direction is chosen for two-fold reasons for our observation of cascade collision: (a) for a smaller simulation box along this direction a cascade collision can occur at a short path, while atom transport by a long-range replacement can be avoided; (b) It will not lead to a tunneling effect. Here primary knock-on energies of 1.69 and 6.0 keV are considered. The simulation is performed at the temperatures of 500K. The computational cell box used at each PKA energy simulation is $20a_0 \times 20a_0 \times 20a_0$, and includes 16000 atoms. $a_0$ is the lattice constant of bcc iron[9]. The simulations of the displacement cascade are carried out for a period of up to 20 ps.

**III. Results and discussions**

We perform the simulation of collision cascade for 20 ps. We find that after about 1.5 ps the system has attained an equilibrium state. At the work of Park et al, such an equilibrium state is reached at about 1.0 ps or so[15]. Present result about the time approaching an equilibrium state is in agreement with one from Park et al's work[15]. For clearly showing the changes of self-interstitials number with collision cascade time, in Fig. 1 we give only out the number of self-interstitials (SIA) as a function of evolution time of collision cascade at the first 6 ps of simulation. In the simulations, if an atom is displaced from its lattice site by at least $0.3a_0$, this atom is considered as an interstitial. In pure bcc iron this criterion has been used by Phythia et al and Yang et al [16].

Fig. 1 (a) and (b) correspond to the PKA energies of 1.69 keV and 6.0 keV, respectively. From Fig. 1 (a) and (b) it can be seen that the collision damage occurs at three stages. For the PKA with energies of 1.69 keV and 6.0 KeV, at the early stage of irradiation, i.e., at the beginning the number of SIA induced by collision cascade increases rapidly with the time of collision, and at about 0.1 ps the number of interstitials approaches a local maximum value. The local maximum number of interstitials is 35 and 41 for PKA energy of 1.69 and 6.0 keV, respectively. After the 0.1 ps the number of interstitials reduces and increases irregularly, and until 0.75 ps number of interstitials approaches 33 and 53 of a local maximum value also for PKA energy of 1.69 and 6.0 keV, respectively. This is an initial stage of collision cascade and lasts about 0.75 ps. At the following time from 0.75 ps to 1.3 ps the number of SIA deduces rapidly. And this corresponds to the second stage of collision cascade. From 1.3 ps to 6 ps of simulation, the number of SIA keeps approximately a constant of 13 for the case with PKA energy of 1.69 KeV and 29 for the PKA energy of 6.0 KeV. The numbers of the SIA keep to the end of the 20 ps simulations for respective PKA energy. This is the third stage of collision cascade. These three stages just correspond to the stage of displaced atom generated by collision cascade, the one of recombination of interstitials and vacancies, and the stage of the dynamical equilibrium of interstitials generation and recombination, respectively. In the first stage a lot of atoms are pushed out of their lattice sites by collision cascade at the given simulation. The second stage indicates that the part of the displaced atoms return to lattice sites after the first stage of collision cascade, i.e., due to a recombination of the interstitials and vacancies the SIA deduces rapidly. After the in-cascade recombination, the cascade damage is determined at its final configuration in bcc iron. From Fig. 1 (a) and (b), it is also seen that the higher PKA energy is, the more inducing defects is. In fact, as shown in the

figures there are some sub-peaks (increases and decrease in the number of interstitials) at the first stage of collision cascade. In the first stage the decrease in the number of interstitials indicates that there is also some recombination of interstitials and vacancies, then the number of SIA increases again and this indicates that the multi-collision cascade produces interstitials again. In the previous works[15-18] the simulations do not reported the process of the recombination and generation of SIA at the initial stage. This maybe is due to that the temperature control is different from each other in present MD simulation and in the previous MD simulations. From Fig. 1 it is found that the irradiation system approaches an equilibrium state at about 1.5 ps. In the work of Park et al[15], they use molecular dynamics to simulate the irradiation damage in tungsten. They find that the number of SIA is about several tens under the PKA energy of 5.0 KeV and the irradiation system approaches an equilibrium state at about 1.0 ps or so[15]. The number of SIA and equilibrium time[15] are in agreement with our present results in Fe, respectively.

In Fig. 2 (a), (b), and (c) we show the simulation results for the traces of collision cascades in bcc iron formed by an iron atom with respective PKA energy of 1.69 keV and 6.0 keV at an incidence index direction of <1 1 0>. In the figure the projection is normal to (010) plane. Fig. 2 (b) is a magnification part of the left bottom in Fig. 2 (a). As shown (for example, see Fig. 2(b)), multiple collision cascades are produced. From our numerical simulations it is found that a displacement cascade proceeds in two steps as it evolves with time. Firstly a balisllistic phase lasts about 0.75 ps, where PKA energy is transferred to many other atoms because of multiple collisions. At the end of a ballistic phase, a central disordered core is created, which consists of a core vacancies surrounded by the associated self-interstitial atoms (SIA). This is the first stage of collision cascade. Subsequently, a thermal-spike phase continues for 0.55 ps, during which most

of the displaced atoms return to lattice sites by a thermal relaxation. This is the second stage of collision cascade. The atoms that fail to regain lattice sites become interstitial atoms, along with vacancies. This is the third stage of collision cascade. These properties are in agreement with the ones by Park et al[15] and Bacon, Gao, and Osetsky [18]. We also find that under the energies of 1.69 KeV and 6.0KeV of PKA the size of the regions where atoms are displaced by the collision cascade are about 11.0 and 15.0 $a_0$, respectively, as shown in Fig. 2(a) and (c). Such a result is not reported in the previous works, such as Ref. 15 and Ref. 18.

From simulated results it can be seen that in the collision cascades, interstitials are produced directly within displacement cascades. We also can find that beside single SIA, there are some defects with isolate dumbbell configuration along <100>, <110>, and <111>. More interesting, we still find the composite defect of <110> and <110> dumbbells, and composite defect of <110> and <111> dumbbells, and they are shown in Fig. 3. In the case of the composite defect, at the corner of a bcc lattice an atom is displaced to some position and becomes a common atom, the atom, its a nearest neighbor atom, and a self-interstitial atom form a composite defect by a combination of <110> and <110> dumbbells, or a combination of <110> and <111> dumbbell (see Fig 3). In the figure, two dumbbells are connected, and their bonding lengths are denoted in Fig. 3, where the bonding lengths are slightly larger than the nearest neighbor distance of 0.2483 nm between Fe atoms. Comparing with a complete lattice, in the figure, the lattice and bond directions are slightly distorted. Using a MD method Yu et al simulate the cascade collision of He in Fe and find that the interstitial dumbbell of Fe–Fe and Fe–He are in the <1 0 0> and <1 1 0> lattice direction[3]. By first principle calculations Fu et al have predicted the existing of the interstitial pair configuration along <110> and <111> in pure bcc iron [17]. Our numerical

calculations about <110> and <100> dumbbells are identical to their theoretical predictions. Using MD simulation Stoller also observe <110> and <111> dumbbell defects in pure Bcc iron [5]. They all do not report a composition defect[5,18].

**IV. Conclusions:**

The structure evolution and nature of defects in bcc iron by collision cascade from molecular dynamics simulation are investigated. Under irradiation, the collision cascade induces not only general defects, such as, self-interstitials, vacancies, <100>, <110>, and <111> dumbbell defects, but also the composite defects, such as the composite defect of <110> and <111> dumbbell, and composite defect of <110> and <110> dumbbell. The collision cascade also gives rise to defect clusters. Simulation shows that the higher the energy of primary knock-on atom is, the more the number of interstitials is. Under considered energy of primary knock-on the size of the regions where atoms are displaced by the collision cascade are about 11-15$a_0$. The smaller the energy of PKA is, the smaller the region is. At the same time, it is also found that even at the initial stage of 0.0-0.75 ps of collision cascade, there is also some combination of interstitials and vacancies.

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**Figures and their captions:**

Fig. 1: The number of self-interstitial atoms produced by collision cascade as a function of evolution time during collision cascade. In the simulations, if an atom is displaced from its lattice site by at least $0.3a_0$, this atom is considered as an interstitial. Figure (a) and (b) correspond to the cases with PKA energy of 1.69 keV and 6.0 keV, respectively, where the higher the PKA energy is, the more the number of interstitials is.

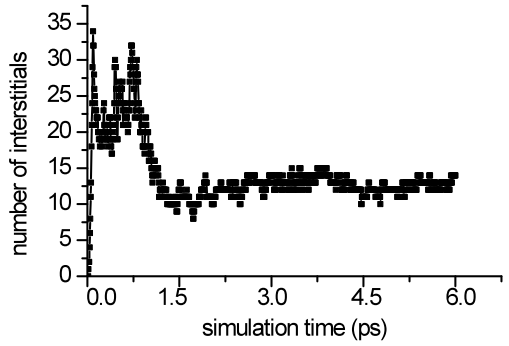


Fig. 1(a)

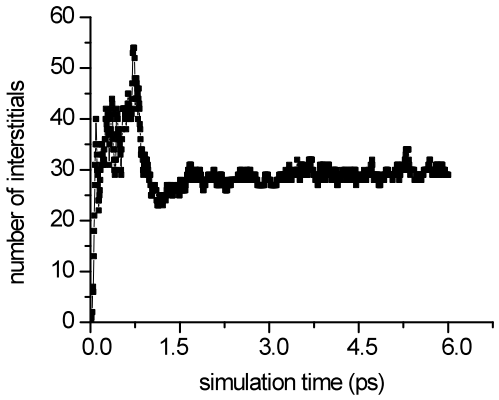


Fig.1 (b)

Fig. 2: (a) and (c) are the traces of collision cascades in bcc iron formed by an iron atom with respective PKA energy of 1.69 keV and 6.0 keV at an incidence index direction of <1 1 0>. In the figure the projection is normal to (010) plane. Multiple collision cascades are produced in the figures and (b) shows a magnification part of the left bottom in Fig. 2 (a).

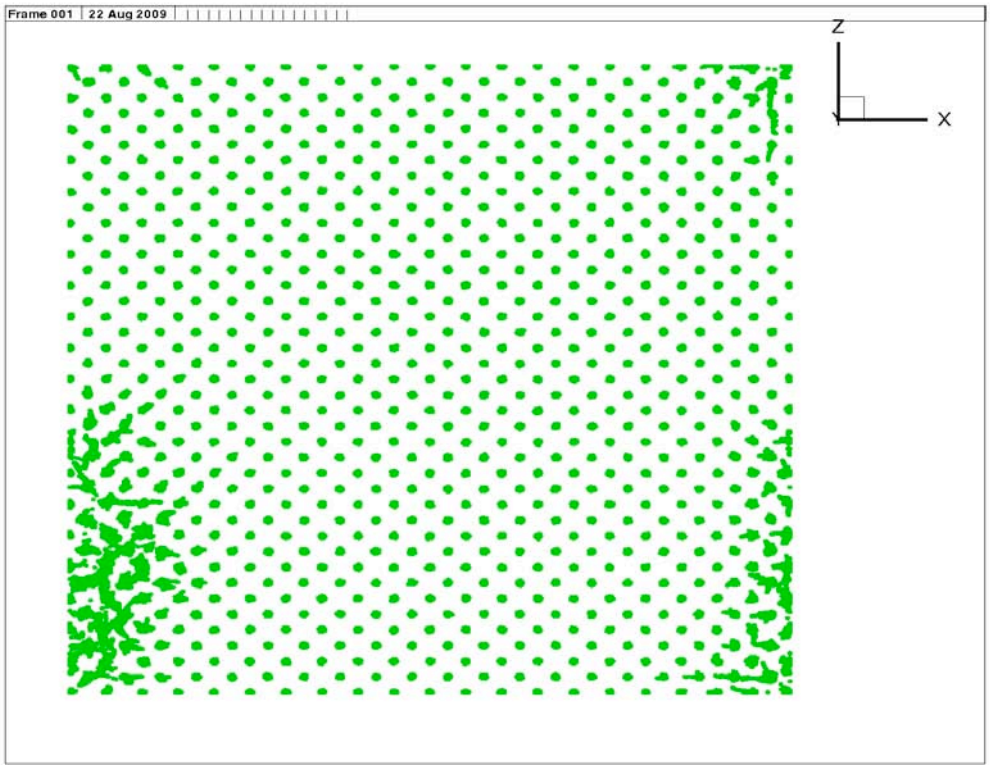


Fig. 2(a)

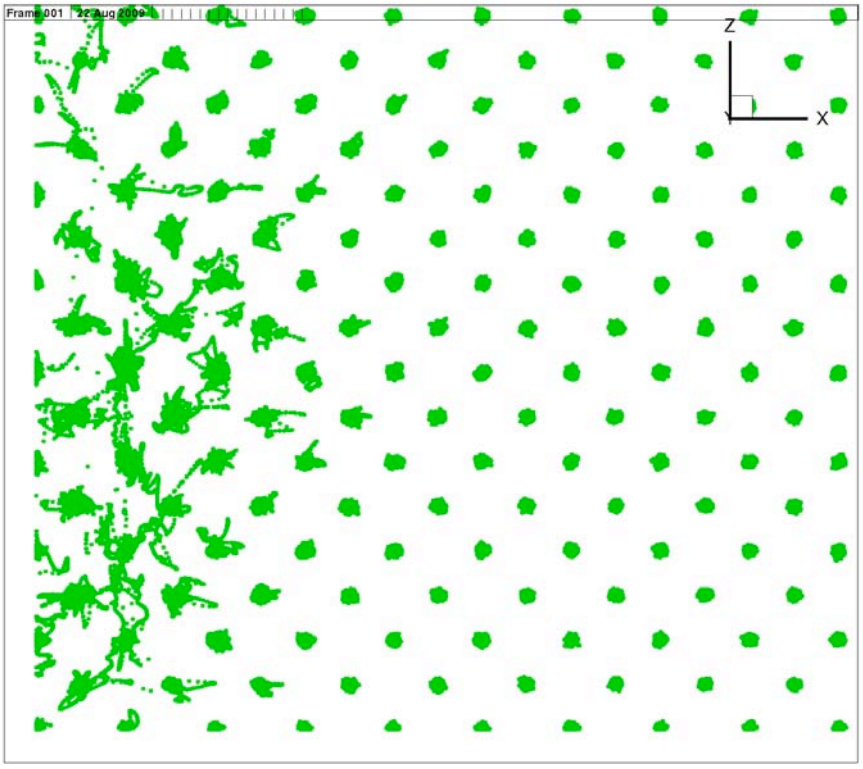


Fig. 2(b)

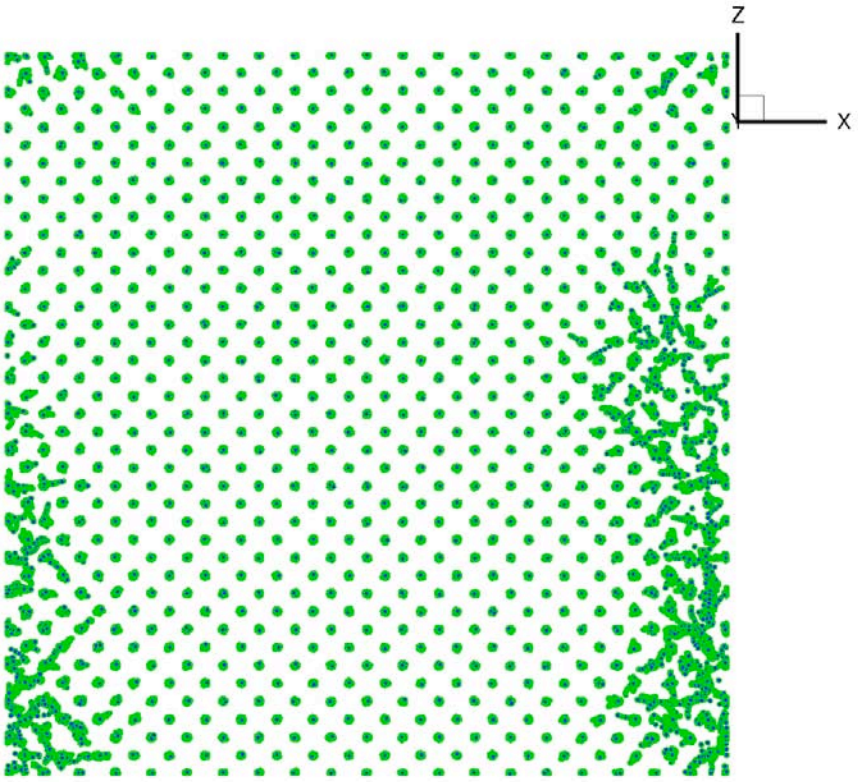


Fig. 2(c)

Fig. 3: The configuration of composite defect, where (a) for the one formed by <110> and <110> dumbbells, and (b) for the one by <110> and <111> dumbbells. In the configuration, at the corner of bcc lattice an atom is displaced to some position; as a common atom, the atom, it's a nearest neighbor atom, and a self-interstitial atom form a composite defect by a combination of <110> and <110> dumbbells, or a combination of <110> and <111> dumbbell. The two dumbbells are connected by dash lines, and their bonding lengths are denoted in the figure. Comparing with a complete lattice, the lattice and bond directions are slightly distorted.

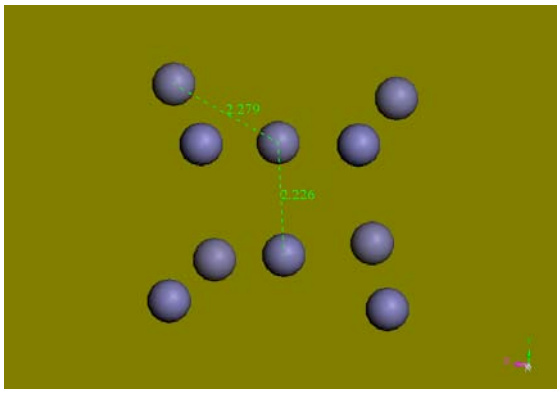


Fig. 3 (a)

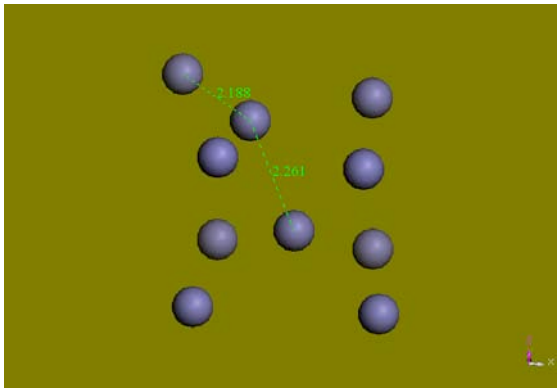


Fig.3(b)