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Keywords

evolution, iron, nanoscale, crack, modelling

Disciplines

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Modelling of the Evolution of Crack of Nano Scale in Iron

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Abstract

Metals own the ability of self-healing to some extent, and the ability of the internal crack healing is most desirable for improving the reliability of metals. A molecular dynamics simulation has been further developed to investigate the evolution of a nano scale crack in body centred cubic Fe crystal under the conditions of heating or compressive pressure. When system temperature drops, the evolution of the crack that was at elevated temperature has been studied for the first time. N-body potential according to the embedded atom method has been adopted. The original nano scale crack is expressed by removing some atoms in the centre of the cell, and the minimum vertical distance between the atoms on the top and bottom crack surfaces has been defined as D_m for assessing the process of crack evolution. The results show that a crack healing process can be accelerated significantly with an increase of temperature. When the system temperature decreases, D_m of the crack that was in healing process does not change significantly but fluctuates in a narrow range. This means that the crack healing is the result of Fe atoms diffusing into the crack area but not the thermal stress incurred in the simulation cell at elevated temperature. The pre compressive pressure under the condition of both biaxial and uniaxial loadings can help promote the crack healing significantly and results in more uniform distribution of defects after healing.

Keywords: Crack, evolution, Iron, heating, compressive pressure

1. Introduction

To some extent, metals own the ability of self-healing. For example, it is well known that a new oxide film can form rapidly on the exposed surface of aluminium or stainless steels to prevent the underlying metals from further oxidation if there is a break over the oxide film. The ability of the internal crack healing in metals is the most desirable to improve the reliability of metals. It is possible that low strength materials might be made more reliable at a low cost if the crack healing is applied at an intermediate stage of their service life. Cracking was not a “reversible” operation, but very small cracks may be healed if the top temperature of the heat-treatment is sufficient to bring the atoms on either side of the crack to within a mutual range by thermal agitation [1]. The self-healing effect for creep cavitation in heat resisting stainless steels has been developed by alloy design, so micro-cracks can be constrained from propagating by automatically forming compounds on the crack surfaces although they may not be annihilated [2, 3].

Quite a few researches have been conducted on crack healing in inorganic and composite materials while less work has been performed on metals. The damage evolution in metals was analysed [4], and many heat treatment methods can be used to reduce the number of defects in metals after a long-term operation at high temperatures [5]. By TEM observation, a crack in α -Fe

was found to be healed completely when the temperature was increased to a critical value of 1073K [6]. It was suggested that the thermal or mechanical treatment provides the driving force to minimise the surface energy resulting in the crack healing [7]. Real internal pre-cracks were obtained in pure copper and steel using plate impact technology [8]. The healing of these cracks was studied in a vacuum at an elevated temperature [9-11], and the inhomogeneous microstructure in crack healing area was also analysed [12]. It has been shown that the healing of fine cracks (100 nm) begins immediately after heating then proceeds according to the vacancy diffusion mechanism in the surface layer about 10 μm thick [13].

The effect of hydrostatic pressure on the shrinkage of cavities in copper introduced by creep at 773 K and situated on grain boundaries was studied [14]. The density of the specimen showed a rapid increase when a hydrostatic pressure was applied during annealing, while the change was little when annealed under atmospheric pressure. The similar result was also obtained in [15]. Sintering of creep-induced grain boundary cavities was carried out in 316 stainless steel by annealed, hot-isostatically pressured and compressive creep at 750 $^{\circ}\text{C}$ [16]. The propagation of damage is restrained in metal during hot deformation, which means that there exists a healing process, while the cracks extend [17]. One of the reasons why the ductility of experimental steels can be improved over the whole working temperature is to annihilate or heal micro-cracks that may occur during deformation [18]. The processes of eutectic phase cracking and the associated processes of crack healing under the action of deformation and temperature in eutectic alloys of the Ti-Al-Si-Zr system have been investigated [19]. The internal crack can be healed completely and rapidly under hot plastic deformation [20]. It is possible to intensify crack healing and/or refinement of the microstructure by adjusting the parameters of plastic deformation or isostatic pressure [21].

From the view of the dissipation structure of physics, it was indicated that the essence of crack healing in materials is a process of exchanging substance and energy for an open system within the environment [22]. Some theories have been suggested to explain the crack healing process. Investigations of the mechanisms of crack opening and healing in a single crystal of commercially pure bismuth showed that both the nucleation and healing of cracks were controlled by twinning [23]. It was suggested that the observed acceleration of the micro-crack healing rate might be associated with the inhomogeneity of the dislocation structure of impulse-deformed crystals [24].

Molecular dynamics (MD) has been adopted to discover the essence of crack healing in metals. MD simulation was conducted to study crack healing in Al [25] and Cu crystals [26], both of which are face centered cubic (FCC). Dislocation generation and motion occur during crack healing. The critical temperature for crack healing depends upon the orientation of the crack plane. Body centered cubic (BCC) crystal is characterised by four close-packed directions, the $\langle 111 \rangle$ directions,

and by the lack of a truly close-packed plane such as the octahedral plane of the FCC lattice. The crack healing behaviour in BCC-Fe crystal during heating has been simulated [27].

However, fixed boundary condition was adopted [27] and one doubt is whether a thermal stress in simulation cell due to restrained thermal expansion acts to close the crack rather than the atom migration resulted from thermal vibration provokes crack healing. In order to clarify the issue, further simulations have been conducted to investigate the behaviour of the crack evolution when the system temperature decreases to room temperature in this study. The effect of temperature on the minimum vertical distance between the atoms on the top and bottom crack surfaces has been obtained. In addition, the evolution of nano scale crack in BCC Fe when there exists a compressive pressure has been investigated.

2. Computational Method

The molecular dynamics method is built based on a set of Newtonian dynamics equations for a number of particles with the macro constraints and boundary condition. They are solved by a numerical method to achieve the classical trajectory and velocity. The macro physical properties and motion routine can be obtained based on the statistical average of the results calculated for a long duration of time.

Assuming the total number of atoms is N , which follows Newton's law.

$$\vec{F}_i = -\frac{\partial U_{tot}(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N)}{\partial \vec{r}_i} = m_i \cdot \vec{\ddot{r}}_i \quad (1)$$

where $i = 1, 2, \dots, N$, U_{tot} is the total potential energy of N atoms, m_i is the atom mass. The position $\vec{r}_i$ and velocity $\vec{v}_i$ of each particle in a system can be obtained by solving Eq. (1). The position $\vec{r}_i(t + \Delta t)$ and velocity $\vec{v}_i(t + \Delta t)$ of each particle at time $t + \Delta t$ depend on the position $\vec{r}_i(t)$ and velocity $\vec{v}_i(t)$ of that particle respectively at time t , and the leapfrog algorithm [28] is applied to calculate the positions and velocities of atoms.

The reliability of the molecular dynamics simulation depends on the description of the inter-atomic potential. The inter-atomic potential adopted here is the N-body potential proposed by Finnis and Sinclair according to the embedded atom method (EMA) [29], and the total energy of an assembly of atoms can be written as

$$U_{tot} = -\sum_{i=1}^N \rho_i^{\frac{1}{2}} + \frac{1}{2} \sum_{j=1}^N \sum_{i=1(i \neq j)}^N V(r_{ij}) \quad (2)$$

where the second term on the right hand side of Eq. (2) is the conventional central pair-potential summation, while the first term is the N-body term, in which

$$\rho_i = \sum_{j=1(i \neq j)}^N \Phi(r_{ij}) \quad (3)$$

where both V and Φ are functions of the inter-atomic distance r_{ij} . Constructed by Ackland et al. [30], the following functional forms have been adopted.

$$\begin{aligned} V(r) &= \sum_{k=1}^6 a_k (r_k - r)^3 H(r_k - r) \\ \Phi(r) &= \sum_{k=1}^2 A_k (R_k - r)^3 H(R_k - r) \end{aligned} \quad (4)$$

Where a_1, a_2, a_3, a_4, a_5 and a_6 are -36.559853, 62.416005, -13.155649, -2.721376, 8.761986 and 100.0000, A_1 and A_2 are 72.868366 and -100.944815, r_1, r_2, r_3, r_4, r_5 and r_6 are 1.180000, 1.150000, 1.080000, 0.990000, 0.930000 and 0.866025 respectively. R_1 represents the cut-off radii of V and R_2 represents the cut-off radii of Φ , which are 1.300000 and 1.200000 respectively [31]. $H(x)$ is the Heaviside unit-step function which gives the cut-off distance of each spline segment.

3. Description of Simulation Cell

3.1 Geometry

The crack that is about 5.957×10^{-9} m long and over $1.500 a_0$ wide ($a_0 = 2.8665 \times 10^{-10}$ m, which is lattice constant of BCC Fe) were expressed by removing some atoms in the centre of the cell [32]. The angle between the $(\bar{1}\bar{1}0)$ slip plane and the crack plane is 60° in this study. The width is larger than the cut-off radii of Φ , $1.300 a_0$, which means that there exists no interplaying force between the atoms on either side of the crack surface. The total number of atoms is nearly 13000. x -axis is along the extension line of the central crack, y -axis along the normal of the crack plane, and z -axis along $[1\bar{1}2]$ direction. The length of the calculation cell along the x -axis direction is $44\sqrt{3} a_0$, y -axis $24\sqrt{2} a_0$, z -axis $\sqrt{6} a_0$. Every three layers of atoms along the x direction constitutes a cycle of $\sqrt{3}/2 a_0$ long, every two layers of atoms along y direction constitutes a cycle of $\sqrt{2} a_0$ long, and every six layers of atoms along z direction constitutes a cycle of $\sqrt{6} a_0$ long.

3.2 Boundary Conditions

The number of atoms in the simulation is usually much less than that in a real system due to huge computation. Boundary conditions have significant effect on the reliability of simulation results. Fixed boundary conditions [33, 34] have been adopted along x and y directions in the simulation at elevated temperature.

The simulation of the behaviour of crack under pre compressive pressure was divided into two stages. Displacement boundary condition and fixed boundary condition [33, 34] have been adopted at the first and second stages of the calculation respectively. At the first stage of the calculation, a

compressive loading was applied on the simulation cell. Displacement boundary condition was adopted along the x and y directions. Both biaxial and uniaxial compressive loadings were taken into account respectively. The boundary atoms have displacement based on the plane strain linear elastic displacement field in the solid containing crack [35]. The configurations at the end of the first stage were adopted as the initial configurations at the second stage and a pre compressive pressure exists in the simulation cell. At the second stage of the calculation, elevated temperature was applied, which starts from 523K then increases at intervals of 50K. Fixed boundary conditions [33, 34] were adopted along x and y directions, which means that the locations of the boundary atoms are constant during the whole calculation process.

In all cases, periodical boundary condition [26, 36] was adopted in z direction. The initial velocity was the Maxwell-Boltzmann distribution corresponding to a given temperature. The system temperature was maintained a constant by scaling the atom velocities during the simulation.

The equilibrium of the original configuration was obtained after a long time relaxing at a low temperature near 0 K, as shown in Figure 1. There exist no defects in this original configuration. D_m is defined as the minimum vertical distance between the atoms on top and bottom crack surfaces and it is used for assessing the process of crack evolution [27]. $D_m = 1.526 a_0$ in the original configuration. Crack healing only becomes possible when D_m is less than the cut-off radii of V , $1.180 a_0$.

Figure 1 Original configuration

4. Results and Discussion

4.1 Effect of temperature when starting from original configuration

The parameters of N-body potentials for BCC Fe are only valid at the temperature below 1185 K. Simulations were carried out in the temperature range of 273 - 1173 K and the increment is 50 K. The simulation spanned 6.0×10^{-11} s and the time step Δt was 1×10^{-16} s.

Relationships between D_m and the time in the temperature from 523 to 923K are shown in Figure 2. It can be seen that D_m experiences a dramatic decrease in the first $1.0 - 2.0 \times 10^{-12}$ s, then increases and tends to fluctuate in a narrow range in all cases. The dramatic decrease may result from the unstable calculation in the first $1.0 - 2.0 \times 10^{-12}$ s. The fluctuation range reduces with an increase of temperature.

Figure 2 D_m vs time at various temperatures starting from the original configuration of Figure 1

When the temperature is 573 K, the fluctuation may be over the cut-off radii of Φ , $R_1=1.300 a_0$. When the temperature is 623 K, the fluctuation range is between $R_1=1.300 a_0$ and the cut-off radii of V , $r_1=1.180 a_0$. When the temperature is 673 K, the fluctuation range is around $r_1=1.180 a_0$. When the temperature reaches 773 or 873 K, the fluctuation ranges decrease rapidly to be around $0.500 a_0$. When the temperature is 923 K, the atoms on top and bottom surfaces move actively as shown in Figure 3, and D_m becomes 0 at 3×10^{-11} s, as shown in Figure 3(d).

The results show that the critical temperature at which the crack healing becomes possible is 673 K. The process of crack healing can be accelerated dramatically when temperature rises. The temperature at which a complete healing may be achieved is 923 K.

Figure 3 Evolution of crack morphology at 923 K

(a) $t = 6 \times 10^{-12}$ s, (b) $t = 1 \times 10^{-11}$ s, (c) $t = 2 \times 10^{-11}$ s, (d) $t = 3 \times 10^{-11}$ s

Figure 4 Evolution of crack morphology at 1173 K

(a) $t = 1 \times 10^{-13}$ s, (b) $t = 1.1 \times 10^{-12}$ s, (c) $t = 1.8 \times 10^{-12}$ s, (d) $t = 4.5 \times 10^{-12}$ s

Figure 4 shows the more rapid process of crack healing at 1173 K. D_m decreases to $0.989 a_0$ at 1×10^{-13} s, which is less than $r_1=1.180 a_0$, shown in Figure 4(a). The crack is separated into two small sections at 1.1×10^{-12} s, shown in Figure 4(b). Only two voids are left at the position of two crack tips after 1.8×10^{-12} s, shown in Figure 4(c) then the crack is healed completely at 4.5×10^{-12} s, shown in Figure 4(d).

4.2 Behaviour of the crack when reducing system temperature

The above simulations were performed in a fixed volume. A thermal stress may occur when temperature is raised as the fixed boundary conditions restrain thermal expansion and it may increases with an increase of temperature. One doubt is whether this thermal stress acts to close the crack rather than the atom migration resulted from thermal vibration provokes crack healing. Further simulations have been conducted to investigate the behaviour of the crack evolution when the system temperature decreases to room temperature.

The initial configurations in this further simulation were actually the configurations in which the crack has experienced the healing process in Section 4.1. Fixed boundary conditions were used along x - and y -axis and periodical boundary condition was in z direction. The room temperature of 293K and the corresponding initial velocity Maxwell-Boltzmann distribution were adopted. The

system temperature was maintained a constant by scaling the atom velocities. The simulation time was up to 6.0×10^{-11} s and the time step Δt was still 1×10^{-16} s.

Figure 5 D_m vs time when temperature decreases to 293K

- A – Starting from the configuration after 5.0×10^{-11} at 573K in the calculation of section 4.1
- B – Starting from the evolved configuration after 1.0×10^{-11} at 923K in the calculation of section 4.1
- C – Starting from the partly healed configuration after 2.0×10^{-11} at 923K in the calculation of section 4.1

Figure 5 shows the relationship between D_m and the time in three typical partly healed configurations when the temperature decreases to 293K. (A) Not healed crack. Crack width in the starting configuration is larger than the cut-off radii of Φ , $R_1 = 1.300 a_0$. (B) Crack in early stage of healing. Crack width in the starting configuration is just less than the cut-off radii of V , $r_1 = 1.180 a_0$. (C) Nearly healed crack. Crack width in the starting configuration has been reduced significantly.

In all cases, D_m does not change significantly but fluctuates in a narrow range in the process. In the case of A, the atoms at top and bottom surfaces were beyond the mutual range in the starting configuration. D_m increases very slightly and fluctuates between 1.3761 and 1.4338 a_0 . In the case of B, the atoms at top and bottom surfaces just fall in the mutual range in the starting configuration. D_m increases slightly and fluctuates around the cut-off radii of Φ , $R_1 = 1.300 a_0$. In the case of C, a large number of atoms at top and bottom surfaces were in the mutual range in the starting configuration. D_m increases firstly then decreases dramatically to the value even smaller than its initial value. The fluctuation range is between 0 and 0.3 a_0 , which is comparatively large. The initial crack morphology and that after 6.0×10^{-11} s at 293K in each case are shown in Figure 6.

Figure 6 Evolution of cracks that have experienced healing process when the temperature reduces
 (a) and (b) initial crack after 5.0×10^{-11} at 573K obtained in section 4.1 and the morphology after 6.0×10^{-11} s at 293K
 (c) and (d) initial crack after 1.0×10^{-11} s at 923K obtained in section 4.1 and the morphology after 6.0×10^{-11} s at 293K
 (e) and (f) initial crack after 2.0×10^{-11} s at 923K obtained in section 4.1 and the morphology after 6.0×10^{-11} s at 293K

4.3 Effect of temperature when pre compressive pressure exists

As described before, this simulation was divided into two stages. At the first stage, the environmental temperature should be low enough to remove the temperature effect, which is 40 K in this simulation. The loading rate that is 0.025×10^{18} Pa m^{1/2}/s has to be many orders of magnitude higher than the real loading rate due to the limitation of the time scale achievable in molecular dynamics. The values of environmental temperature and loading rate here are not specific and can

be variable in a reasonable range without incurring significant difference in the following calculation.

The simulation was realized by adopting the same methodology used in sections 4.1 and 4.2. The only difference is that the displacement boundary conditions corresponding to biaxial and uniaxial loading conditions were adopted along x and y directions respectively instead of the fixed boundary condition. The boundary atoms have displacements based on the plane strain linear elastic displacement field in the solid containing crack [35], i.e.

$$\begin{cases} u_x = \frac{1+\nu}{E} \{[(1-2\nu)\text{Re}\bar{Z}_I - y\text{Im}Z_I] + [2(1-\nu)\text{Im}\bar{Z}_{II} + y\text{Re}Z_{II}]\} \\ u_y = \frac{1+\nu}{E} \{[2(1-\nu)\text{Im}\bar{Z}_I - y\text{Re}Z_I] + [(2\nu-1)\text{Re}\bar{Z}_{II} - y\text{Im}Z_{II}]\} \end{cases} \quad (1)$$

where u_x , u_y are the displacements in x and y direction respectively, E is Young's modulus, ν is Poisson's ratio. Z_I and Z_{II} are Westergaard functions. $Z_I = \sigma/\sqrt{1-(a/z)^2}$. Z_{II} is 0 in the case of biaxial loading while it is $-i\frac{\sigma}{2}$ in the case of uniaxial loading, in which σ is the applied stress, a is the half length of the central crack. $Z(z) = d\bar{Z}(z)/dz$ and $z = x + yi$. Equation (1) was achieved in continuum mechanics and has been successfully applied in molecular dynamics calculation [6, 25, 26].

The simulation starts from the original configuration shown in Figure 1. The time step is Δt is 1×10^{-15} s and the total simulation time in this first stage is 1.018×10^{-11} s. The configurations under the conditions of biaxial and uniaxial compressive loadings after 1.018×10^{-11} s are shown in Figure 7. In the case of biaxial compressive loading, $D_m = 1.505 a_0$, as shown in Figure 7(a). In the case of uniaxial compressive loading, $D_m = 1.492 a_0$, as shown in Figure 7(b).

Figure 7 Configurations under the condition of compressive loading after 1.018×10^{-11} s
(a) biaxial, (b) uniaxial

These two simulation cells were introduced into the second stage as the initial configurations for studying the effect of temperature, which means a pre-compressive pressure exists in the simulation cells.

Figure 8 D_m vs time at various temperatures starting from the configurations under pre compressive pressure

(a) starting from the configuration after biaxial compressive loading, (b) starting from the configuration after uniaxial compressive loading

Figure 8 shows the relationships between D_m and the time at the temperature from 523 to 873K. The results in both cases are similar. When the temperature is 523K, D_m fluctuates in the narrow range between $R_1=1.300 a_0$ and the cut-off radii of V , $r_1=1.180 a_0$, which means the crack cannot be healed. When the temperature rises to 573K, D_m decreases dramatically to be less than the cut-off radii of V , $r_1=1.180 a_0$. This means the critical temperature at which the crack healing becomes possible is 573K when the pre- compressive pressure is applied. It is 100K lower than the critical temperature at which the crack can be healed starting from the original configuration shown in Figure 1.

Comparing the results in Figure 8 with those in Figure 2, it can be seen that the existence of compressive pressure is not only helpful for reducing the required temperature for crack healing but also can significantly promote the crack healing process. In Figure 2, D_m fluctuates around the cut-off radii of V , $r_1=1.180 a_0$ when the temperature is from 523 to 673K. It fluctuates around $0.5-0.7 a_0$ when the temperature is from 723 to 873K. In Figure 8, D_m fluctuates around $0.6 a_0$ or below when the temperature reaches only 573K. In the temperature of 573 - 773K, the fluctuation range basically does not move down with an increase of temperature, which is different from the results shown in Figure 2. The only exception appears in the healing process at 773K starting from the configuration obtained after the uniaxial compressive loading. In this case, D_m decreases rapidly to $0.6 a_0$ after 1×10^{-11} s then fluctuates around $0.3 a_0$.

Whether the simulation starts from the original configuration shown in Figure 1 or the configurations under pre- compressive pressure, the cracks can be completely healed when the temperature reaches 923K.

During the compressive loading at the first stage of calculation, atoms deviates from their normal positions in some area, which results in defects circled in Figure 9. It is inferred that the existence of these defects prompts the crack healing process.

Figure 9 Defects in part of the simulation cell after the compressive loading of 1.108×10^{-11} s
(a) biaxial compressive loading, (b) uniaxial compressive loading

Figure 10(a) and (b) show some defects in crack healing region and the surrounding area after 6.0×10^{-11} s at 1173K starting from the configurations with pre compressive pressure. The dashed rectangle frames show the locations of the original crack. Defects can be found to appear in the whole simulation cells and their positions are random. This seems different from the situation that the defects aggregate in the crack healing region when the original configuration of Figure 1 is adopted [27], which means the existence of the defects in the simulation cell after compressive loading are helpful for generating more uniform distribution of defects after crack healing.

Figure 10 Distribution of defects after 6.0×10^{-11} s at 1173K

(a) starting from the configuration under biaxial compressive loading, (b) starting from the configuration under uniaxial compressive loading

Essentially, the crack itself can be considered a very large defect in the simulation cell. The existence of the crack results in extra surface energy then increases system energy. There is a tendency to eliminate the crack to reduce the system energy. However, the crack healing process cannot happen when the temperature is low because an energy barrier exists between the states when the crack exists and when the crack is healed. Rising temperature to activate atoms can help overcome the energy barrier. The activated atoms close to crack immigrate into the crack area and vacancies appear in the positions from where atoms emigrated, then the atoms adjacent to these vacancies need to adjust their positions. Crack size is much larger than the size of any other defects appearing in the simulation cell. It may cost much more time for those atoms immigrating into the crack area to rearrange their positions than the atoms that just need adjust their positions to accommodate adjacent vacancies. This may be the reason why the distribution of defects is not uniform in the early stage of healing.

The healing of a crack means that a huge defect evolves into a lot of small defects and all the defects may not be eliminated. However, the atoms have to adjust their positions continuously in order to reduce the system energy even after the crack has been healed. This continuous position adjustment results in more uniform distribution of defects with an increase of time, and the quantity of the defects in the crack area will be reduced. The existence of the defects in the simulation cell may accelerate the process of the position adjustment after crack healing.

5. Conclusions

The evolution of the nano scale cracks in BCC Fe crystal has been simulated using molecular dynamics. In the case that there exist no defects in the original configuration, the critical temperature at which crack healing becomes possible is 673 K. A complete healing may be achieved in 6.0×10^{-11} s at 923 K. Temperature has a significant effect and crack healing process can be significantly accelerated with an increase of temperature. When system temperature decreases, the size of the crack that was in the different stages of healing process does not change significantly but fluctuates in a narrow range. The crack healing is the results of Fe atoms diffusing into the crack area, but not the thermal stress incurred in the simulation cell due to the adoption of fixed boundary conditions. The effects of pre compressive pressure generated under the condition of both biaxial and uniaxial loadings after 1.018×10^{-11} s have been studied. The pre compressive pressure is not

only helpful for reducing the required temperature for crack healing but also can significantly promote the crack healing process. The distribution of defects is generally uniform under the condition of pre compressive pressure while more defects aggregate in the healing area when starting from the original configuration.

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Figure captions

Figure 1 Original configuration

Figure 2 D_m vs time at various temperatures starting from the original configuration of Figure 1

Figure 3 Evolution of crack morphology at 923 K

Figure 4 Evolution of crack morphology at 1173 K

Figure 5 D_m vs time when temperature decreases to 293K

Figure 6 Evolution of cracks that have experienced healing process when the temperature reduces

Figure 7 Configurations under the condition of compressive loading after 1.018×10^{-11} s

Figure 8 D_m vs time at various temperatures starting from the configurations under pre compressive pressure

Figure 9 Defects in part of the simulation cell after the compressive loading of 1.108×10^{-11} s

Figure 10 Distribution of defects after 6.0×10^{-11} s at 1173K

Figure 1 Original configuration

Figure 2 D_m vs time at various temperatures starting from the original configuration of Figure 1

Figure 3 Evolution of crack morphology at 923 K
(a) $t = 6 \times 10^{-12}$ s, (b) $t = 1 \times 10^{-11}$ s, (c) $t = 2 \times 10^{-11}$ s, (d) $t = 3 \times 10^{-11}$ s

Figure 4 Evolution of crack morphology at 1173 K

(a) $t = 1 \times 10^{-13}$ s, (b) $t = 1.1 \times 10^{-12}$ s, (c) $t = 1.8 \times 10^{-12}$ s, (d) $t = 4.5 \times 10^{-12}$ s

Figure 5 D_m vs time when temperature decreases to 293K

A – Starting from the configuration after 5.0×10^{-11} at 573K in the calculation of section 4.1

B – Starting from the evolved configuration after 1.0×10^{-11} at 923K in the calculation of section 4.1

C – Starting from the partly healed configuration after 2.0×10^{-11} at 923K in the calculation of section 4.1

Figure 6 Evolution of cracks that have experienced healing process when the temperature reduces

(a) and (b) initial crack after 5.0×10^{-11} s at 573K obtained in section 4.1 and the morphology after 6.0×10^{-11} s at 293K
(c) and (d) initial crack after 1.0×10^{-11} s at 923K obtained in section 4.1 and the morphology after 6.0×10^{-11} s at 293K
(e) and (f) initial crack after 2.0×10^{-11} s at 923K obtained in section 4.1 and the morphology after 6.0×10^{-11} s at 293K

(a)

(b)

Figure 7 Configurations under the condition of compressive loading after 1.018×10^{-11} s
 (a) biaxial, (b) uniaxial

(a)

(b)

Figure 8 D_m vs time at various temperatures starting from the configurations under pre compressive pressure

(a) starting from the configuration after biaxial compressive loading, (b) starting from the configuration after uniaxial compressive loading

Figure 9 Defects in part of the simulation cell after the compressive loading of $1.108 \times 10^{-11} \text{s}$

(a) biaxial compressive loading, (b) uniaxial compressive loading

(a) (b)
Figure 10 Distribution of defects after 6.0×10^{-11} s at 1173K

(a) starting from the configuration under biaxial compressive loading, (b) starting from the configuration under uniaxial compressive loading