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EFFECT OF TEMPERATURE ON DISLOCATION EMISSION FROM CRACK TIP FOR BCC METAL MO*

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ABSTRACT The effect of thermally activated energy on the dislocation emission from a crack tip in BCC metal Mo is simulated in this paper. Based on the correlative reference model on which the flexible displacement boundary scheme is introduced naturally, the simulation shows that as temperature increases the critical stress intensity factor for the first dislocation emission will decrease and the total number of emitted dislocations increase for the same external load. The dislocation velocity and extensive distance among partial dislocations are not sensitive to temperature. After a dislocation emission, two different deformation states are observed, the stable and unstable deformation states. In the stable deformation state, the nucleated dislocation will emit from the crack tip and piles up at a distance far away from the crack tip , after that the new dislocation can not be nucleated unless the external loading increases. In the unstable deformation state, a number of dislocations can be emitted from the crack tip continuously under the same external load.

KEY WORDS correlative reference model, flexible displacement boundary, molecular dynamics, dislocation emission, temperature

I. INTRODUCTION

In the study of mechanical behavior near the crack tip, temperature plays a crucial role which has been attracted the attention of many researchers. Various brittle-to-ductile transition (BDT) models have been proposed based on experimental or calculation results. Both the elastic and atomistic methods have been used to investigate the nucleation and emission of dislocations. But the effects of thermal activation on the process of dislocation emission have not been well considered. The experimental results of Samuels and Roberts[1] and Chiao and Clarke[2] concerning the temperature dependence of the mechanical behavior of crystal show that there is a transition temperature, below which the fracture is brittle and above which the fracture is ductile. It is shown by Brede and Haasen[3] and Brede[4] that very sharp brittle to ductile transition takes place in a temperatuer range of a few Celsius degrees for material Si and the transition temperature increases with increasing loading rate.

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The activation energy for dislocation nucleation from a stressed crack tip was calculated by Rice and Beltz[4] with in the Peierls framework in which a periodic shear stress versus displacement relation is assumed to be held on a slip plane. In their work, the energy required to thermally activate a stable, incipient dislocation into its unstable 'saddle-point' configuration was calculated with the asymptotic method in 2-D and 3-D. The effect of thermal activation is very significant in reducing the applied load for dislocation emission. By combining the molecular dynamics (MD) simulation results of mode I crack tip with a dislocation mechanics analysis, Cheung et al. [5] extended Rice-Thomson model[6] and calculated an activation barrier of the nucleation of a half-square dislocation loop on a specific orientation of BCC crystal (α-Fe). The effects of material softening due to stress and temperature were obvious in their analysis.

The molecular dynamics simulation using the Morse potential carried out by Mullins[7] shows that at low temperature the crack propagates as a brittle cleavage crack, while at high temperature the crack is blunted by the emitting dislocation. The calculation of molecular dynamics by Kitagawa and Nakatani[8] shows that there is a linear relation between the thermal activation energy and temperature. Based on Rice and Thomson model[9], Li considered the thermal activation energy as a function of the energy release rate[10]. Applying the 3-dimensional MD method for FCC crystal Cu, Zhang et al. [11] simulated the effect of thermal activation on the nucleation and emission of dislocation, and proposed an explicit relation between the critical condition of dislocation emission and temperature. But the fixed displacement boundary scheme was used in their simulation which results in a serious deficiency, the emitted dislocations being incapable of penetrating the border of the molecular dynamics simulation cell.

A correlative reference model and the flexible displacement boundary scheme have been proposed by Tang and Wang[12]. Following the work[12], the effect of temperature on the dislocation emission from a crack tip for BCC Mo crystal is studied in this paper with the MD method. The emitted dislocation can penetrate the border smoothly as the flexible displacement boundary offers no resistance to the dislocation motion. It is convenient to analyze the interaction between the crack and the emitted dislocation. Four cases of different temperatures of 50K, 120K, 200K and 300K are analysed in our simulation. By referring to the works of Kitagawa et al. [8], Li[10] and Zhang et al. [11], an explicit relation between the critical stress intensity factor and temperature is proposed. This relation is in good agreement with our molecular dynamics results.

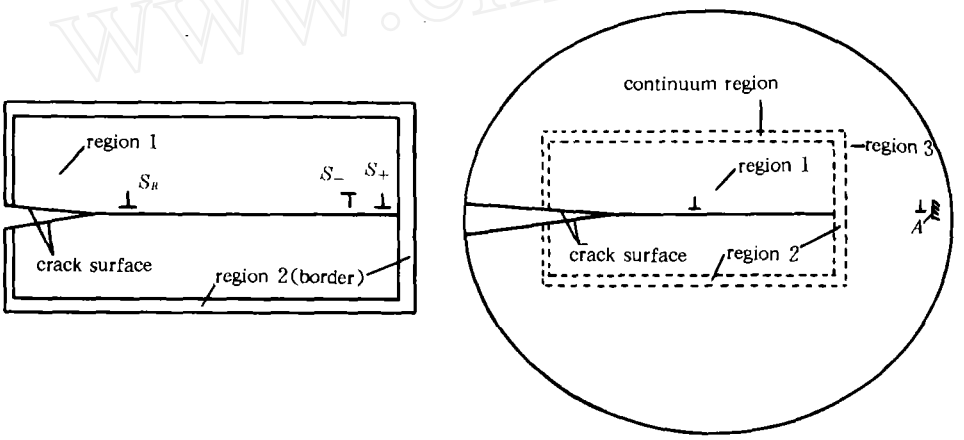
Ⅱ. MECHANICAL MODEL

The correlative reference model is schematically shown in Fig. 1. Figure 1(a) shows a simulated sample of MD approach with a single edge crack. The region 1 is the inner discrete atoms, and region 2 is the border of inner simulated atoms. S_R represents an emitted dislocation. Figure 1(b) shows an infinite continuum with a semi-infinite single edge crack, whose elastic constants, such as E, μ, ν, are the same as those of the simulated crystal Mo. The geometric configuration and the size outlined by the dotted line in Fig. 1(b) are also the same as those of Fig. 1(a). This infinite elastic continuum is designated as a reference model and subjected to remote loading.

There is a correlation between the simulated sample and the reference model. Two requirements must be satisfied in the simulation.

(1)The displacement of the atoms in region 2 in Fig. 1(a) is imposed by the displacement of the corresponding region in the reference model.

(2)Supposing that there are N_T dislocations emitted from the crack tip, with $N_T = N_1 + N_3$. The positions of the N_1 emitted dislocations in region 1 of Fig. 1(b) are defined by the discrete atomic configuration in Fig. 1(a). Other N_3 dislocation positions in the continuum region 3 are determined by the dislocation pileup theory of mesomechanics.



(a) Schematic diagram for the simulated sample

(b) Schematic diagram for the infinite continuum with a single edge crack

Fig. 1 Schematic diagram for the correlative reference model.

Consider the problem of the reference model, the pure K_{I} stress field is prescribed at infinity and the stress intensity factor K_{I} is chosen as a load parameter. Suppose the slip plane is coincident with the crack plane and the slip direction is along the x axis in the present study. Hence all emitted dislocations lie on the x axis. Based on the linear elastic theory, the displacement field of the infinite continuum with a single semi-infinite edge crack and N_T discrete dislocation is given by the following equation:

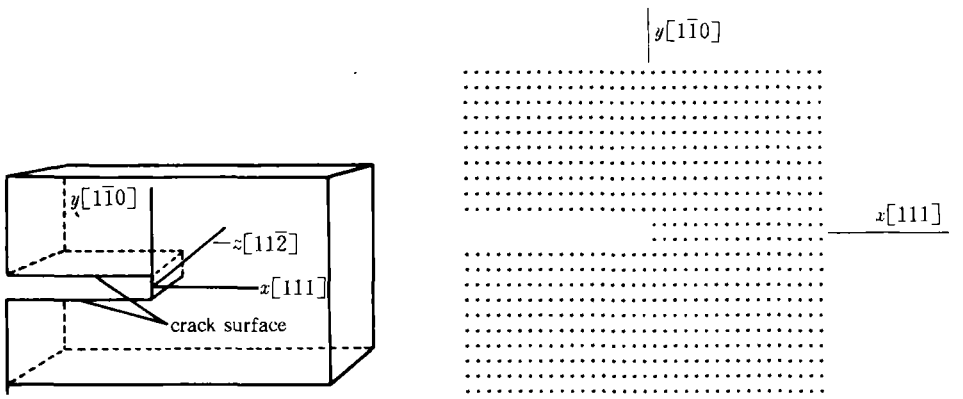
$$u_l = u_l^A + \sum_{i=1}^{N_T} u_l^D(x, y; x_i) \tag{1}$$

where l represents coordinate components in x and y directions, x_i is the position of the i-th discrete dislocation, both u_l^A are u_l^D are the displacement fields corresponding to the applied remote load and to the dislocation respectively, The displacement u_l depends not only on the applied remote load but also on the emitted dislocation. For detailed description of the correlative reference model see paper [12].

Ⅲ. CALCULATION METHOD

3.1 Crack Tip Geometry

The parallelepiped with a slit is used as the simulation model in which the slip plane is coincident with crack plane ($\theta = 0^0$). The coordinate system is selected to be x, y and z axes along $[111]$, $[1\bar{1}0]$, $[11\bar{2}]$, respectively. As shown in Figs. 2(a), 2(b), the size of the atomic area is $500\times\frac{\sqrt{3}}{6}a_0$ in x direction, $40\times\frac{\sqrt{2}}{2}a_0$ in y direction and $6\times\frac{\sqrt{6}}{6}a_0$ in z direction. Along x direction, the periodicity is in three layers of (111) atomic planes and its length is $3\times\frac{\sqrt{3}}{6}a_0$; along y direction, the periodicity is in two layers of $(1\bar{1}0)$ atomic plane and its length is $2\times\frac{\sqrt{2}}{2}a_0$; along z direction, the periodicity is six layers of $(11\bar{2})$ atomic plane and its length is $6\times\frac{\sqrt{6}}{6}a_0$; the left side of boundary to the crack tip is $120\times\frac{\sqrt{3}}{6}a_0$; the separation of the upper and lower crack planes is taken to be $\sqrt{2}\,a_0$; the number of atoms in the present model is about 20000. Figure 2(b) shows the atomic arrangement of six adjacent $(11\bar{2})$ planes projected on the same layer.



(a) Schematic diagram for simulation model

(b) The initial positions of atomic arrangement near crack tip region, six layers of $(11\bar{2})$ planes projected on the same plane

Fig. 2 Crack tip geometry in BCC metal Mo.

3.2 Interatomic Potential

The N-body potential constructed by Tang et al. [13] is used in this paper.

3.3 Boundary Condition

The flexible displacement boundary scheme explained in section 2 is applied here. Along z-direction, the periodic boundary condition is adopted. But the atoms in the present simulation sys-

tem can move in z-direction because of the six layers of $(1\bar{1}2)$ atomic planes adopted.

3.4 Calculating Method

The leapfrog algorithm[14] is used in this paper. The loading rate is $\dot{K}_I = 0.0706$ (MPa • $m^{1/2}$/ps), and the stress intensity factor K_I is chosen as the loading parameter. The time step is 1.256×10^{-14}s.

3.5 Temperature Condition

All atoms in the simulation area are assigned the initial velocities derived from a Maxwellian velocity distribution corresponding to a given temperature. The isothermal process is required during the simulation. Suppose that the simulation system is connected to a big heat reservoir at a certain temperature which provides sufficient heat energy to maintain the system at a fixed value throughout the duration of the runs. This means that any small disturbance due to the loading increment or dislocation emission can be neglected[14,15].

Ⅳ. RESULTS AND DISCUSSION

The positions of a full dislocation versus time for the case of $T = 50$K are plotted in Fig. 3 in which little dots represent the positions of partial dislocations associated with the emitted dislocations. A full dislocation is dissociated into three partial dislocations in BCC crystal Mo. Because the curve of the dislocation positions versus time is nearly a straight line beyond the distance of $5a_0$ from a crack tip from which the dislocation velocity can be derived easily and is a constant, about 1800m/s～1950m/s. Three partial dislocations of the first full dislocation have been nucleated as $t = 9.5$ps and $K_{Ie} = 0.668$MPa • $m^{1/2}$.

The results in Figs. 4(a), (b), (c) correspond to the case of $T = 120$K. There are altogether three full dislocations (9 partial dislocations) emitted and the time interval of dislocation emission is not homogeneous according to scale time in the unit of ps, which are 21ps and 4ps respectively. Combining Fig. 4(a) with Fig. 4(b), we can see that as $K_I = 0.64$MPa • $m^{1/2}$, three partial dislocations of the first full dislocation have been nucleated. Compared with the case of $T = 50$K, the critical stress intensity factor for the first full dislocation emission decreases about 4.2%. After penetrating through the border the first full dislocation is assumed to pile up $5000a_0$ from the crack tip. The interaction between the first full emitted dislocation and crack tip results in a reduction of stress field around the crack tip and makes the discrete atom system be in stable deformation state in which the new dislocations can not be nucleated from the crack tip unless the system is loaded again. Because there is no dislocation in the region of MD, the discrete atom system should be loaded again at the same loading rate as before.

When K_I reaches 0.73MPa • $m^{1/2}$, the deformation of the discrete atom region is in an unstable state in which more than two full dislocations can be emitted continuously as the external loading is to be kept unchanged. The second and third full dislocations have been observed at the same stress level of 0.73MPa • $m^{1/2}$ in Fig. 4(a) and Fig. 4(b). The simulation shows that the discrete atom system experiences two different deformation states corresponding to two different external stress levels respectively at a temperature of 120K. This example clearly shows that

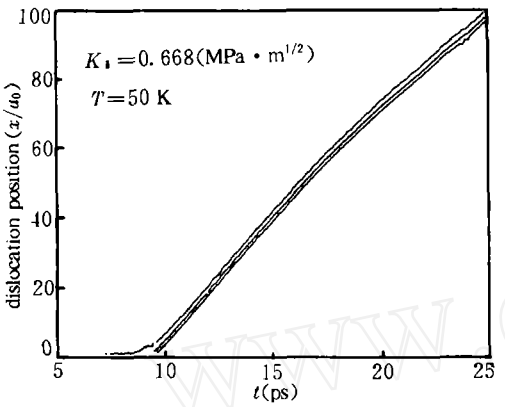


Fig. 3 Emitted dislocation position versus time.

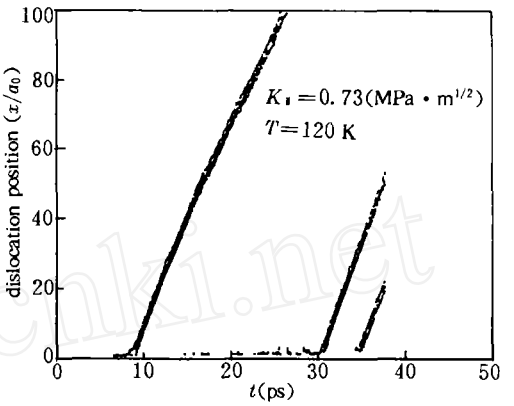


Fig. 4(a) Emitted dislocation position versus time.

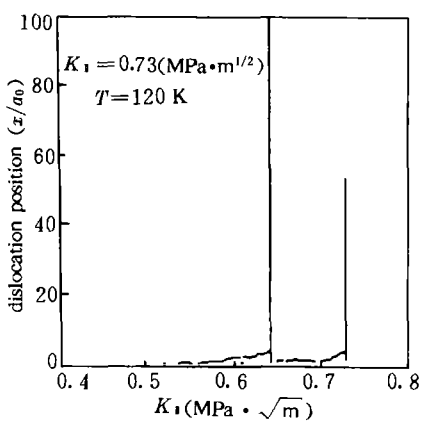


Fig. 4(b) Emitted dislocation position versus applied stress intensity factor.

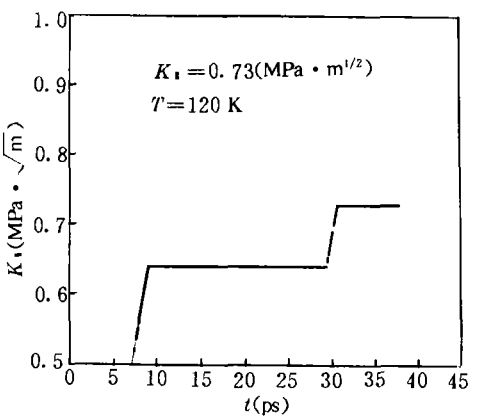
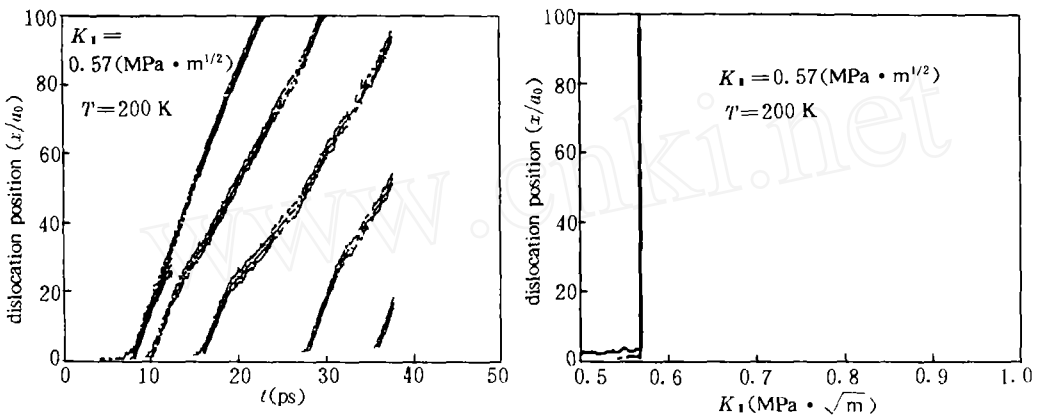


Fig. 4(c) Applied stress intensity factor versus time.

when the external load reaches a certain stress level, the discrete atom system can be in an unstable deformation state.

For the case of $T=200$K, the first full dislocation has been emitted as $K_I=0.57$MPa • $m^{1/2}$. Compared with the case of $T=120$K, the critical stress intensity factor for the first full dislocation emission is reduced. It can be seen from Fig. 5(a) that, as $t=4$ps, the first partial dislocation has been nucleated, It does not move away, but still hovers around the crack tip until $t=8$ps, while three partial dislocations of the first full dislocation are nucleated and move away quickly from the crack tip. We pause to load temporarily, keep the load unchanged, and relax the discrete atom system. After about 2ps, the second three partial dislocations are emitted. The space between the first and second full dislocations is about $15a_0 \sim 20a_0$. As the distance from a crack tip is within $20a_0$, the velocities of the second and third full dislocations are nearly the same as that of the first full dislocation. But as the distance is over $25a_0$, the velocities of the second and third full dislocations are reduced. The reason is that as emitted dislocations are far away from the crack tip, the interaction between the dislocation and crack tip becomes less violent, but

the interaction between two neighbouring dislocations is the same as before, so the latter interaction appears more important. The second full dislocation is subjected to the repulsive force from the first full dislocation. The same analysis also applies to the third full dislocation.

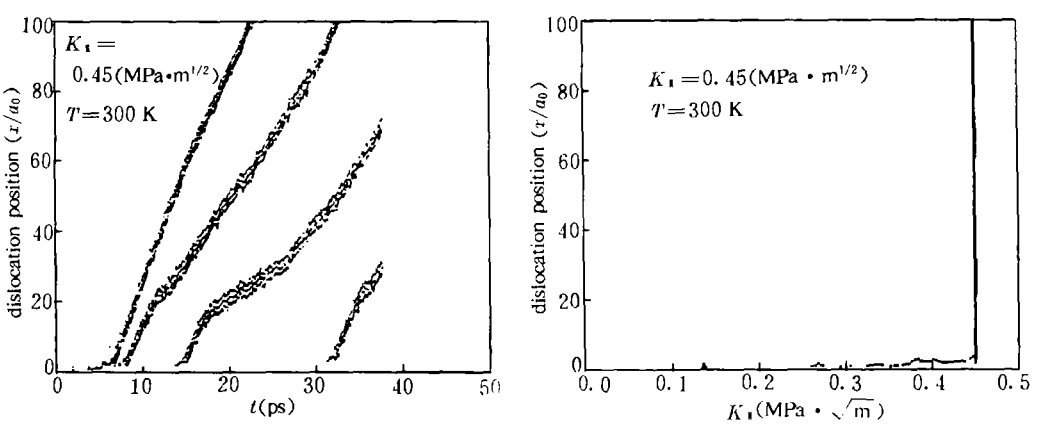


(a) Emitted dislocation position versus time

(b) Emitted dislocation position versus the stress intensity factor

Fig. 5

Combining Fig. 5(a) with Fig. 5(b), we can see that altogether five full dislocations (15 partial dislocations) have been emitted at a stress level of 0.57MPa • m$^{1/2}$ temperature of 200K. The discrete atom system does not experience the stable deformation state but reaches the unstable deformation state directly at a low stress level. The effect of temperature on the dislocation emission and deformation state is obvious. The phenomenon of the discrete atom system reaching the unstable deformation state directly is also observed for the case of T = 300K as shown in Fig. 6 (a) and Fig. 6(b).



(a) Emitted dislocation position versus time

(b) Emitted dislocation position versus the stress intensity factor

Fig. 6

The above analysis may apply to the case of $T=300$K and the same result can be obtained. As the temperature increases, the total number of the emitted dislocations will increase greatly for the same stress level.

For the case of $T=300$K, the critical stress intensity factor K_{I_e} for the first full dislocation emission is reduced to 0.45MPa • $m^{1/2}$ which is less than 20% that of the case of $T=200$K. Similar to the case of $T=200$K, the simulated system reaches the unstable deformation state directly. Four full dislocations (12 partial dislocations) have been observed at the same stress level $K_{\mathrm{I}}=0.45$MPa • $m^{1/2}$ as shown in Fig. 6(a) and Fig. 6(b). From recent simulation of MD, we can obtain the conclusion that as the temperature increases, the velocity of the first full dislocation is almost the same, about 1800m/s～1950m/s. This means that the dislocation velocity is not sensitive to the temperature. But the effect of interaction of dislocations on the dislocation velocity is obvious and may greatly affect the average velocity of dislocation array .

The shear stress along the prolongation of crack plane is shown in Fig. 7 at a load level of $K_{\mathrm{I}}=0.45$MPa • $m^{1/2}$ and $T=300$K. The positions of two full dislocations are about $30a_0$ and $70a_0$ reapectively. It can be seen that our result is in good agreement with that of the elastic solution. The curve of stress distribution in molecular dynamics is in the form of wave which is contributed by the thermal vibration of discrete atoms.

Dislocation emission from a crack tip depends on both the stress and temperature. At temperature TK, both the activation energy of dislocation emission ΔG and the critical stress intensity factor $K^0_{\mathrm{I}_e}$ were given by Li[11] i. e.

$$\Delta G = Ab^2\left(\ln\frac{2Ab}{K_{\mathrm{I}_e}}\sqrt{\frac{2\pi}{r_0}}-1\right) \tag{2}$$

$$K^0_{\mathrm{I}_e} = \frac{2Ab}{e}\sqrt{\frac{2\pi}{r_0}} \tag{3}$$

where e is the base for natural logarithm, r_0 the core cutoff of dislocation, A is $\frac{\mu}{2\pi(1-\nu)}$ for the edge dislocation, μ the shear modulus, ν the Poisson's ratio and b the Burger's vector of the dislocation. $K^0_{\mathrm{I}_e}$ is the critical stress intensity factor for the first full dislocation emission corresponding to 0K.

Since the dislocation emission is a thermally activated process, the critical condition for dislocation emission will be reduced by the thermal activation. The simulation of MD by Khantha et al.[16], Kitagawa et al.[8] and Zhang et al.[11] shows that the activation energy $\triangle G_T$ is in a linear relation with temperature. Hence it is assumed that the relation between activated energy and temperature T is given by

$$\triangle G_T = \frac{2\alpha K_B T}{b} \tag{4}$$

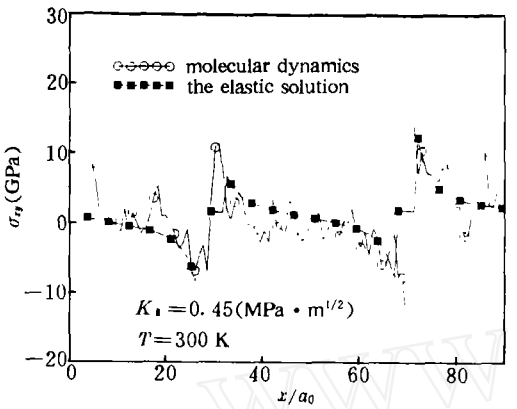


Fig. 7 Shear stress distribution along the prolongation of the crack.

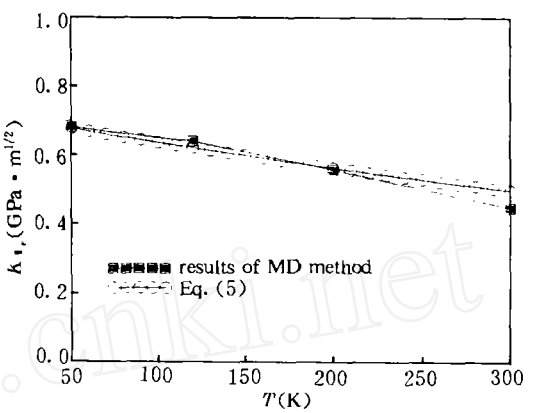


Fig. 8 The critical stress intensity factors versus temperature.

where $\triangle G_T$ is the thermally activated energy per unit length of the dislocation, α is the parameter related to the material and loading rate and K_B is Boltzmann's constant.

The activation energy barrier of dislocation emission reduces $\triangle G_T$ which is contributed by the temperature T. Thus we can obtain the critical condition for dislocation emission at temperature T.

$$K_{I_e}^T = K_{I_e}^0 \exp\left(-\frac{2\alpha K_B T}{Ab^3}\right) \tag{5}$$

where $K_{I_e}^T$ is the critical stress intensity factor for the first full dislocation emission corresponding to TK. If the simulated result of MD in the case of $T = 50$K is taken as a reference value, the critical condition at any temperature can be derived from Eq. (5). The result of Eq. (5) and the MD result are shown in Fig. 8. It can be seen that they are in good agreement. Here $\alpha = 99$.

V. CONCLUSIONS

Based on the correlative reference model and the MD simulation, this paper studies the dislocation emission from the crack tip under the condition of various temperatures. The main results concerning the effect of temperature on the process of dislocation emission are summarized as follows.

(1) As the temperature increases, the critical stress intensity factor for the first full dislocation emission decreases, and the total number of the emitted dislocations for the same external load tends to increase. When the emitted dislocations are far away from the crack tip, the interaction between dislocations becomes more violent which greatly affects the average velocity of dislocation array.

(2) The extensive distance among the partial dislocations and the velocity of each single full dislocation is not sensitive to temperature change.

(3) For the BCC Mo, the simulation result of the critical stress intensity factor for the first emitted full dislocation versus temperature in MD method is in good agreement with that of the simple analysis given by Eq. (2).

(4) In the dislocation emission process, generally, there are two deformation states, the stable and unstable. As the temperature is higher than 200K, the simulated system reaches the unstable deformation state directly at the lower external load.

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