DISLOCATION EMISSION AND EQUATION OF ENERGY BARRIERS AT MODEL I CRACK TIP①

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ABSTRACT The propagation for the model I crack in aluminum single crystal has been directly studied by *in-situ* TEM observation. The equation of energy barrier of the dislocation building-up and emission at the model I crack tip has been established by means of Peierls-Nabarro dislocation model and starting from angle of energy. By means of calculation, the critical value of spontaneous emission of the dislocations from tip of the model I crack was obtained.

Key words emission of dislocation propagation of crack Peierls-Nabarro dislocation model energy barriers model I crack

1 INTRODUCTION

Studying the changes of the material microstructure near the crack tip dynamically and the effects to the material fracture processing is very important, which has aroused great interests of quite a lot of scholars[1-5]. As we know, some scholars have observed that by various experiments the cracks of the loaded solid materials can emit dislocations when the load comes to a certain value. So they have raised a lot of different theories and models to research the physical conditions of the dislocations emission, but almost all of them used the method of stress analysis on the basis of the dislocations locating somewhere of the crack tip without considering the process of its gradual forming. In the stress analysis, they didn't consider the interaction force among the dislocations and the lattice resistance while the dislocations were moving, moreover, when the dislocations are quite near the crack tip (within the lattice constant), owing to the interactions among the atoms and the complication of the environment, it is very difficult to describe clearly its properties and states by the force equilibrium. In this paper, by Peierls-Nabarro dislocation model, in the dimension of the atom, the dislocation's building-up and emission at the model I crack tip under the two-dimension were researched from the angle of energy, the equations of the process were established, and the quantitative criteria of the dislocation emission were built by numerical value calculation.

2 EXPERIMENT MATERIALS AND PROCEDURES

The material used in the experiment was aluminum single crystal, pureness 99.999%, ground below 0.05 mm, then sprayed on the ZYS-P Ⅱ double spraying electrolysis polishing instrument, made into the specimen as shown in Fig. 1. In the experiment we installed the specimen on the SEH table, by the JEM-100CX Ⅱ Transmission Electron Microscope, *in-situ* observed the dynamic tensile at the room temperature with the tensile rate of 0.05～1 μm/s and the tensile load of 4.9 N.

After the specimen was loaded, the main crack propagated continuously at the crack tip (namely in the area of the double spraying

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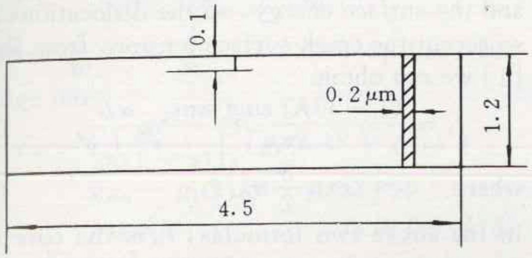

Fig. 1 Geometry and size of specimens (in mm)

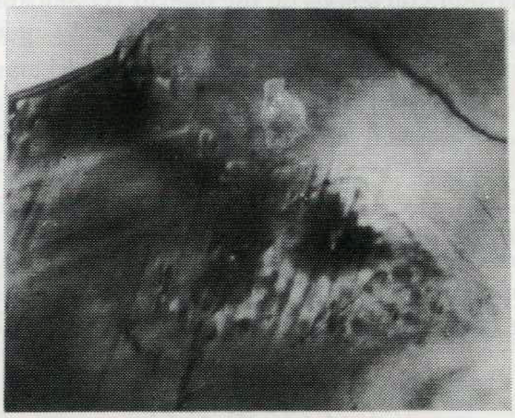

Fig. 2 Dislocation emission from crack tip, ×48 000

pole), during the process, numerical dislocations along the glide plane were emitted constantly from the crack tip, as shown in Fig. 2, there we could see not only the dislocations emitted from the crack tip, but also glide lines which were along the fixed angle with the crack. This showed that during the crack propagation, model I crack tip could emit dislocations just like model Ⅱ and model Ⅲ cracks. After the load stopped, the dislocations emission didn't stop until the stress relaxation reached a degree. At the same time, the crack passivated gradually. During the passivation we could find that the area of dislocation emission went forward from the crack tip and stopped emission gradually, formed the dislocation free zone.

3 ENERGY EQUATION OF DISLOCATION EMISSION BY CRACK TIP

In the process of crack propagation, the crack emitted the dislocations constantly. Rice and Thomson[1], Ohr[2] analyzed it in theory; they considered that the emitted dislocations accepted three forces: image force (σ_i), surface tension (σ_l) and repulsive force (σ_e) produced by the outside stress strength factor. Obviously here were neglected two important aspects: one is that the dislocations emitted outside must overcome the lattice resistance, $\sigma_{P\text{-}N}$ force, the other is that we should also consider the interactions among the dislocations.

3.1 *Dislocation Self Stress* σ_s

When the model I crack was loaded, the dislocations were emitted along the glide plane in an algle of 45 degree with the crack, as shown in Fig. 3. The dislocations plane roused the relative movement of atom face above and below the glide plane, this shift could be described by infinite small dislocations on the glide plane, whose densites are

$$D(r)=\begin{cases}0 & (r\leqslant 0)\\ \dfrac{b}{\pi}\dfrac{w}{(r-l)^2+w^2} & (r>0)\end{cases} \quad (1)$$

where l is the distance from the dislocation centre to the crack tip, w is the dislocation width. According to the dislocation theory[8], the interaction force produced by the infinite small dislocations on the plane of $R=0$ is

$$\sigma_S(r)=\frac{\mu}{2\pi(1-\nu)}\int_0^\infty \frac{D(s)}{r-s}\mathrm{d}s \quad (2)$$

where s is medium variable, put (1) into (2), then

$$\sigma_s(r)=\frac{\mu b}{2\pi(1-\nu)}\frac{1}{(r-l)^2+w^2}[(r-l)\times \left(\frac{1}{2}+\frac{1}{\pi}\mathrm{arctg}\,\frac{l}{w}+\frac{w}{2\pi}\ln\frac{r^2}{l^2+w^2}\right)] \quad (3)$$

where μ is material shear modulus, ν is Poisson ratio, b is Burgers vector.

3.2 *Dislocation Image Force* σ_i

Fig. 3 shows that the dislocations accepted the image force σ_i coming from the free plane (namely crack), suppose that the semilength of crack is C, on the base of Hassen and Leibfried[9] and Rice and Thomson[1], We get

$$\sigma_i(r) = -\frac{(2\sqrt{2}-1)\mu b w}{4\pi(1-\nu)\sqrt{r}} \times \frac{1}{\sqrt{l^2+w^2}\sqrt{\sqrt{l^2+w^2}-l}} \quad (r>0) \tag{4}$$

where $\sigma_i(r)$ is the image force along the radius direction, and the negative sign indicates the direction of the crack tip.

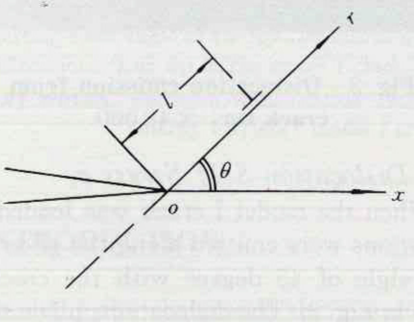

Fig. 3 Dislocation near the model I crack tip

3. 3 *Repulsive Force Field By Load*

The load produced a stress field around the crack tip. The dislocations (Fig. 3) accepted the repulsive force as follows:

$$\sigma_e(r) = \frac{K_I}{\sqrt{8\pi r}} \sin\theta \cos\frac{\theta}{2} \tag{5}$$

where K_I is the stress strength factor.

3. 4 *The Lattice Resistance (Peierls-Nabarro Force)*

The dislocations emitted from the crack tip accept the lattice frictional force, namely lattice resistance, which is

$$\sigma_{P\text{-}N}(r) = \frac{2\mu}{1-\nu}\exp\left[-\frac{2\pi a_1}{(1-\nu)b_1}\right] \tag{6}$$

where a_1 is the distance between the glide planes, whereas b_1 is the atom distance along the glide direction.

3. 5 *Surface Tension f_l and Stress Field σ_l*

After the dislocations were emitted from the crack tip, there formed a step in the crack tip, which increased the areas of the crack tip and the surface energy, so the dislocations also accept the crack surface tension, from Ref. [1] we can obtain

$$f_l = \frac{(1-\nu)K_I^2 \sin\theta \sin\varphi}{2\pi\mu}\frac{\alpha b}{r^2+\alpha^2} \tag{7}$$

where $\alpha = (\exp\frac{3}{2})r_0/2$, (8)

In the above two formulas, r_0 is the core radius of the dislocation, θ is the included angle between crack plane and glide plane, φ is the angle between Burgers vector and forward position of crack. From eq. (7), we can know the stress field produced by f_l is

$$\sigma_l(r) = \frac{f_l}{b} = \frac{(1-\nu)K_I^2 \sin\theta \sin\varphi}{2\pi\mu}\frac{\alpha}{r^2+\alpha^2} \tag{9}$$

3. 6 *Energy Equation of Dislocation Emission*

Because the dislocations accept five forces during its emissions, we can calculate the energy of the dislocation emission. By analysis, we know that the energy of the dislocation emission involves two parts, one is the elastic energy (E_{el}) on the two half infinite crystals of unit length coming from the dislocation emission, the other is the atom malposition energy (E_m) of the two atoms near the emitted plane.

According to the Peierls model, the atom misfit energy is

$$E_m = \frac{\mu b^2}{4\pi(1-\nu)}\left(\frac{1}{2}+\frac{1}{\pi}\text{arctg}\frac{l}{w}\right) \tag{10}$$

whereas the elastic energy can be got as follows by the force conditions

$$E_{el} = 2\left\{\frac{1}{2}\int_0^\infty [\sigma_i(r)-\sigma_s(r)]u(r)\mathrm{d}r + \int_0^\infty [\sigma_l(r)+\sigma_{P\text{-}N}(r)-\sigma_e(r)]u(r)\mathrm{d}r\right\},\ r>0 \tag{11}$$

In the equation above, the first integral factor 1/2 is owing to $\sigma_i(r)$ and $\sigma_s(r)$ which are built gradually during the dislocations building-up, while $\sigma_l(r)$, $\sigma_{P\text{-}N}(r)$ and $\sigma_e(r)$ keep unchangeable during this period, $\mu(r)$ is the bit shift of atom planes above and below the glide plane produced by dislocation emission, which is

$$\mu(r) = \frac{b}{4} - \frac{b}{2\pi}\text{arctg}\frac{r-l}{w} \quad (12)$$

Suppose $\frac{r}{w} = s$, $\frac{l}{w} = \lambda$, then eq. (11) can change into

$$E_{el} = \frac{\mu b^2}{2\pi(1-\nu)}\int_0^\infty [g_i(s,\lambda) + g_I(s) + g_{P\text{-}N} - g_s(s,\lambda) - g_e(s)] \times \mu(s,\lambda)ds \quad (s > 0) \quad (13)$$

thus, the total energy is

$$E_T = E_{el} + E_m \quad (14)$$

After engaged in dimensionless treatment for eq. (14), we can turn it into

$$\overline{E}_T = \frac{E_T}{\frac{\mu b^2}{2\pi(1-\nu)}} = \int_0^\infty [g_i(s,\lambda) + g_I(s) + g_{P\text{-}N} - g_s(s,\lambda) - g_e(s)]u(s,\lambda)ds + (\frac{1}{4} + \frac{1}{2\pi}\text{arctg}\lambda) \quad (s > 0) \quad (15)$$

Eq. (15) is the equation of energy barrier which discribes the dislocation emission from the model I crack tip. In the equation above each item can be substituted

$$g_i(s,\lambda) = (2\sqrt{2} - 1)/(2\sqrt{s}\sqrt{1+\lambda^2} \times \sqrt{\sqrt{1+\lambda^2} - \lambda}) \quad (16)$$

$$g_e(s) = \frac{(1-\nu)^2 K_I^2 \sin\theta \sin\varphi}{\mu^2 b} \times \frac{\beta}{s^2 + \beta^2} \quad (17)$$

In eq. [17], $\beta = [\exp(3/2)](s_0/2)$, $s_0 = r_0/w$

$$g_{P\text{-}N} = \frac{8\pi w}{b}\exp(-\frac{2\pi a_1}{(1-\nu)b_1}) \quad (18)$$

$$g_s(s,\lambda) = \frac{1}{1+(s-\lambda)^2}[(s-\lambda)(\frac{1}{2} + \frac{1}{\pi}\text{arctg}\lambda + \frac{1}{2\pi}\ln\frac{s^2}{1+\lambda^2})] \quad (19)$$

$$g_{(e)}(s) = \frac{2k_I(1-\nu)}{\mu b}\sqrt{\frac{2\pi w}{S}} \quad (20)$$

4 VALUE RESULTS OF ENERGY EQUATION AND ANALYSIS

After the energy equation is put mathematical shift, we can get the standard energy $\overline{E}_T$, here are two parameters: A and λ, $A = K_I(1-\nu)\sqrt{2\pi w}/(\mu b)$, which is connected with the load; while $\lambda = l/w$, which is connected with the place of the dislocation centre. Put the parameters of the Al single crystal: $\mu = 27\,000$ MPa, $\nu = 0.347$, $E = 66\,621$ MPa, $b = 2.86$ nm into the equation, we can acquire that under the different load A, energy $\overline{E}_T(\lambda)$ changes with the value λ, as shown in Fig. 4.

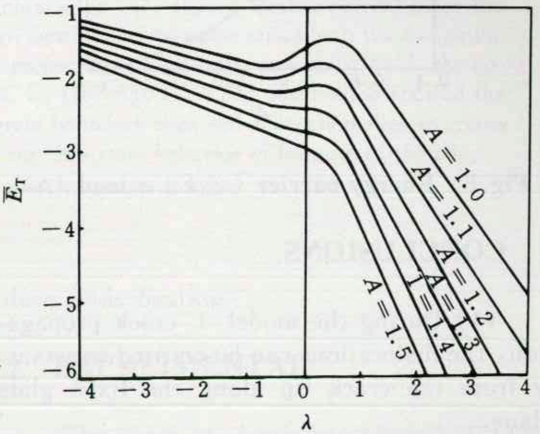

Fig. 4 $\overline{E}_T$ *vs* λ **while** $A = 1.0 \sim 1.5$

Fig. 4 also shows that when the load is lower, there are one minimum value and one maximun value in the curve $\overline{E}_T$-λ; the gap between them is the energy barrier ($\triangle E$) which resists the dislocations emission. When $\lambda < 0$, it is shown that the dislocations have not formed completely. From Fig. 5, we also find that the energy barrier ($\triangle E$) decreases gradually with the increases of the load A. When the load reaches a critical value $A_C = 1.318$, $\triangle E = 0$ (Fig. 5), the dislocations can be emitted from the crack tip automatically without resisting the energy barrier, the criterion is

$$\overline{K}_{IC} = 1.318\frac{\mu b}{(1-\nu)\sqrt{2\pi w}} \quad (21)$$

We compare the results with those of the Schoeck model Ⅲ crack, the critical load of the model Ⅰ crack is bigger; in other words, the model Ⅰ crack tip emits dislocations more difficulty, which agrees with the facts.

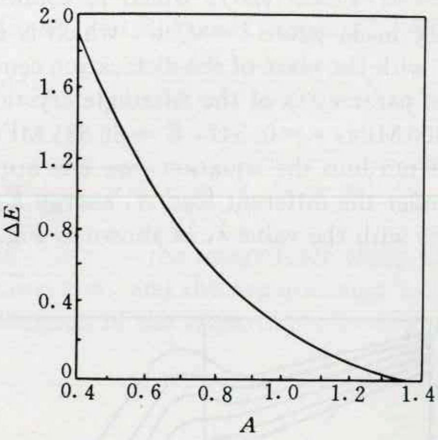

Fig. 5 Energy barrier ($\triangle E$) *vs* load (A)

5 CONCLUSIONS

(1) During the model Ⅰ crack propagation, the dislocations can be emitted constantly from the crack tip along the fixed glide plane.

(2) When the dislocations are emitted from the crack tip, they overcome the resistance of the energy barrier, which decreases with the increase of the load; when the load reaches a critical value, the dislocations can be emitted from the crack tip automatically.

(3) For the aluminum single crystal, the critical load of the dislocation emission is $\overline{K}_{IC} = 1.318\mu b/[(1-\nu)\sqrt{2\pi w}]$.

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