M-9 On the Mechanism of Cleavage Fracture of Crystals

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Abstract

Based on an idea that ductility of perfect lattice, that is, counterbalance of nucleation of cleavage crack and dislocation loop at high stress level, may play important roles in the initiation and propagation of cleavage crack, some calculations were presented for the activation energies of nucleation of crack and dislocation loop, and their consequences were pursued on the plastic work associated with the propagation of cleavage cracks. It was suggested that nucleation of dislocations at the tip of crack may be the primary factor controlling the plastic work in fast propagating cleavage cracks at high temperatures.

§ 1. Introductions

In the previous theories presented so far for cleavage fracture of crystals, emphasis has been laid mainly on the behaviours of pre-existing dislocations, for instance, stress concentration caused by piling up of dislocations,[1] or stress relaxations due to movement of dislocations at the edge of propagating crack.[2][3]

In these theories, therefore, lattice resistance of dislocation, density of pre-existing dislocations[3] and also rate of multiplication of dislocations[4] have been considered to be important measures for ductility of crystals.

On the other hand, experimental evidences show that the ductility of whiskers, dislocation free crystals, depends on easiness of nucleation of dislocation,[5] that the propagation of cleavage crack was in many crystals arrested by dislocations nucleated at the tip of crack,[6] and also that dislocations are rather easily nucleated at various stress concentrated regions.

These evidences suggest that the stability of crystal lattice, i.e. nucleation of crack or dislocation loop in perfect lattice, is another important factor in the criterion of ductility of crystals at most in atomistic dimentions.

There seems to be no exact calculation method for this problem at the present time though it is considered to be a fundamental one. In this paper, however, we shall attempt some preliminary discussions on this problem[7] including their consequences on the mechanisms of initiation and propagation of cleavage cracks.

§ 2. Criterion of ductility of crystals at $0^{\circ}K$.

The criterion of ductility of crystals which are strained homogeneously at $0^{\circ}K$ was in principle provided by M. Born[8] in his theory of stability of crystal lattice. The criterion may be stated in a convenient form that; a crystal may cleave or deform plastically according as the ratio $\beta = \tau_{th}/\sigma_{th}$, a constant characteristic to the crystal, is larger or smaller than the ratio $\alpha = \tau_{max}/\sigma_{max}$, a constant characterizing the state of applied stress, where σ_{th} and τ_{th} are the critical normal stress of separation and the critial shear stress of plastic deformation of the crystal lattice, and τ_{max} and σ_{max} are the components of applied stress corresponding to τ_{th} and σ_{th}

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respectively. Some calculations are illustrated for stress-strain relations of Lennard Jones type crystals under the tensile and pure shear strainings in Figs. 1 and 2.

On the other hand, the stress-strain relation has a close connection with the Peierls' stress through the structure of core of dislocation. Some calculations based on the generalized Peierls' approximation which was developed in the previous paper[9] are illustrated in Fig. 3, it may be noted that the Peierls' stress is very sensitive for small variations in shear stress-strain relation.

§ 3. Criterion of ductility of crystals at finite temperatures

At finite temperatures, however, the criterion of ductility of crystals are governed by the relative magnitude of the probabilities of nucleation of crack and dislocation. The same method of analysis as proposed for the Peierls stress presented above, can also be applied to activation energies of nucleation of two-dimensional crack or dislocation pair. In this paper, however, simple calculations are illustrated for these quantities assuming appropriate sinasoidal laws for tensile or shearing stress-strain relations. For instance, the tensile stress-strain relation of a crystal is approximated in the form,

$$\sigma=\sigma_{th}\sin\frac{2\pi u}{\lambda}\quad,\quad \lambda=\frac{2\pi a\sigma_{th}}{E}\quad,$$

as shown in Fig. 4b, then we obtain the activation energy[1] for nucleation of two-dimensional crack, Fig. 5a, as

$$U_{c2}=\frac{G a^2}{2\pi(1-\nu)}\left(\frac{2\pi\sigma_{th}}{E}\right)^2 log\left(\frac{\sigma_{th}}{\sigma_\infty}\right).$$

On the other hand, for the case of dislocation pair, we must take into account successive nucleations of partial dislocation pairs and stacking fault between them when the dislocation can split, where the activation energy is determined by that of first stage, i.e. the nucleation of a partial dislocation pair, in the case of F.C.C. metals, while the processes are more complicated in B.C.C. metals. The present approximation, therefore, can only be applied to the cases, for instance, the first stage in the case of F.C.C. metals and the nucleation of twin dislocation pair or the complete dislocation pair in the case of B.C.C. metals.

Then by using appropriate assumptions the approximate formulas for three-dimensional cases can be calculated as shown in Figs. 5b and 6, and written in the forms,

$$\begin{aligned} U_c &\simeq \frac{\sqrt{6}\,G\,a^3}{8\pi(1-\nu)(1-\nu^2)}\left(\frac{2\pi\sigma_{th}}{E}\right)\left(\frac{\sigma_{th}-\sigma_\infty}{\sigma_{th}}\right)^{1/2},\\ U_s &\simeq \frac{\sqrt{6}\,G\,b^3}{4\pi(1-\nu)^2}\left(\frac{2\pi\tau_{th}}{G}\right)^2\left(\frac{\tau_{th}-\tau_\infty}{\tau_{th}}\right)^{1/2}, \end{aligned}\qquad (1)$$

when σ/σ_{th} and τ/τ_{th} are nearly equal to 1, where U_c and U_s are the activation energies for nucleations of crack and dislocation loop (half-dislocation loop and stacking fault layer in the case of F.C.C. metals), E, G and ν Young's and rigidity modulus and Poisson's ratio respectively, a the spacing of nearest atomic planes of cleavage, b the distance of nearest

[1] The calculation is based on the method presented by Nabarro[10] for the case of dislocation pair, but recalculated in this paper because his calculation contained some mistake as pointed out by Read.[11]

atomic planes of slip. Some numerical examples are illustrated in Tables. 1 and 2.

It is noted that these formulas predict much smaller values for the activation energies than those calculated by Griffith's theory for U_c, Fig. 5b and Table 1, and Frank and Cottrell's[12] for U_s, Fig. 6 and Table 2. This means that the thermal nucleation of crack and dislocation under high stress are considered to be the processes easier than those suggested in the former theories.

§ 4. Applications of the theories to propagation of cleavage crack.

The theories stated above are then applied to the problem of growth of plastic work associated with the steady propagation of cleavage crack. While macroscopic condition of the propagation of crack is described by the Mott's equation,[13] the conditions for the progress of cleavage crack and the growth of plastic work associated with it may be given by the microscopic conditions at the tip of propagating crack. And when the velocity of crack is not very near to that of shear wave, the processes of propagation may be described as a rate process, that is, at finite temperatures dislocation loops may be nucleated ahead of the crack together with cracks. On the other hand, the dislocation loops may spread in the stress field neighbouring the tip of crack with the velocity which depends on the mobility of dislocation.

At first the condition of the propagation of cleavage crack is expressed by that of successive nucleation of cleavage crack all over the edge of propagating crack, that is,

$$n_c\times 2d^2=1$$

$$n_c=\frac{1}{V}\nu\alpha' N^{1/3}\exp-U_c/kT,\quad U_c=k_c(\sigma_{th}-\sigma_{max}),\qquad (2)$$

where n_c is the number of cracks nucleated per unit area, $2d^2$ the area of one nucleated crack, U_c the activation energy of nucleation of a crack at the edge of propagating crack as assumed in the form presented above, σ_{max} the operative maximum stress at the tip of crack at finite temperature, σ_{th} the cleavage stress at the tip of crack at 0°K, V the velocity of propagation of the crack, ν the frequency of atomic vibration, N the number of atoms per unit volume, α' a number nearly equal to 1.

On the other hand, the plastic work per unit area of the crack W is expressed by,

$$W=2n_s q$$

$$n_s=\frac{1}{V}\nu\alpha' N^{1/3}\exp-U_s/kT,\ U_s=k_s(\tau_{th}-\tau_{max}),\qquad (3)$$

where n_s is the number of loops nucleated per unit area, and q the plastic work caused by the spreading of one dislocation loop in the stress field ahead of the propagating crack, U_s the activation energy of nucleation of a dislocation loop at the edge of the crack, τ_{max} the operative maximum resolved shear stress in the direction and on the plane of a slip system at the tip of propagating crack at finite temperature, and τ_{th} the corresponding theoretical stress.

On the mobility of dislocation, many factors have been investigated on it's velocity and temperature dependencies, for instance, Peierls' stress, non-linear effect of core of dislocation when the velocity is near to that of shear wave,[14] scattering of sound wave, phonon viscocity, and also

effect of dispersed impurities, but few reliable data are available over wide range of velocity and temperature.[15] We shall therefore only adopt for the present the form

$$v = C_t \exp -\frac{E}{kT}, \quad E = A \log \frac{\tau_p}{\tau}, \qquad (4)$$

where v is the velocity of dislocation, and C_t that of shear wave. Then, estimating ϕ by means of appropriate assumptions for the spreading of dislocation loop as explained in Fig. 7, and combining (2) and (3) we obtained the result;

$$\log_{10}\left(\frac{W}{K\tau_{max}b}\right) = 3\log_{10}\left(\frac{\tau_{max}}{\tau_p}\right) + \frac{3kT}{A}\log_{10}\left(\frac{2C_t}{v}\right) + \alpha\frac{k_s}{k_c}\log_{10}\left(\frac{V}{2d^2\nu\alpha' N^{1/3}}\right)$$
$$+ \log_{10}\left(\frac{\nu\alpha' N^{1/3}b^2}{V}\right) - k_s\sigma_{th}(\beta-\alpha)/kT\log_e 10. \qquad (5)$$

The first two terms on the right hand side of the equation (5) represent the contribution of mobility of dislocation, and the last three terms the contribution of brittleness of crystal lattice.

Then in order to estimate the terms in eq. (5) for the cases of LiF, Fe and Cu, which are representative ones of brittle, semi-brittle and ductile materials respectively, the available experimental values for these crystals are listed in Table 3. Those for LiF were taken from the papers of Gilman.[15][16] τ_{max}/τ_p in Fe was estimated from our experiment[17], and A in Fe was deduced from the activation energy of Bordoni's peak in Nb,[18] and A in Cu from the Bordoni's experiment.[19] Since cleavage crack is stopped at 300°K in Fe where the value of W is about $10^{4\sim5}$ C.G.S., we took the representative vaue of W as 6×10^4, and $K\simeq 1/2$, $\tau_{max}\simeq G/20 = 4\times10^{10}$C.G.S., and also $b\simeq 3\times10^{-8}$ C.G.S. in the case of Fe, and estimated the value of left hand side of eq. (5) as $(\log_{10} W/K\tau_{max}b) = 2$. And the same value of the left hand side term was assumed for the case of LiF at 300°K.

Then using the values in Table 3, the terms in right hand side of eq. (5) were estimated and listed in Table 4. The terms underlined —— were calculated using eq. (5), the term underlined ═ was assumed, the third terms in eq. (5) were neglected as small quantities, and also we assumed $\nu\alpha' b/2C_t \simeq 1$.

Other factors which contribute to plastic work, for instance pre-existing Frank-Read sources or Cottrell locking, were then examined, and the results showed that these factors were really important when the speed of crack and also temperature were rather low,[3] but not essential factors compared with the one estimated above when the velocity of crack and temperature were rather high. Main reasons for the deductions were that, at first the number of sites of multiplication of dislocations, such as F.R. sources and sites of double cross slip is more limited, secondly the time required for the multiplication of dislocations is consequently longer, and thirdly the activation energies for the processes of multiplication are larger, or the processes are more insensitive for temperature excepting that of lattice resistance, compared with those of nucleation of dislocations at the tip of cracks in the critical cases stated above.

Although our estimation of Table 4 is no more than a tentative one because of much unknown factors particularly of the mobility of dislocation at high velocities, we may draw out from it some qualitative conclusions. For instance, if we assume the limiting value of $(\log_{10} W/K\tau_{max}b)$ where cleavage is able to be maintained be 3, our estimations presented in Table 4 predict higher critical temperature for propagation of cleavage crack for LiF

compared with those of Fe and Cu. This seems to provide a qualitative explanations for the experimental evidences that, the arresting temperature of propagation of brittle fracture in iron is known to be about 400°K,[20] single crystal of LiF shows brittle fracture even at temperature near the melting point of 1116°K in Charpy test,[21] and no cleavage is found on Cu.

§ 5. Discussion

1) Present study was started based on the idea that the cleavability of crystals may essentially be the intrinsic characteristic of crystal lattice at high stress level, then the criterion for stability of crystal lattice, i.e. counterbalance of nucleation of crack and dislocation loop, may be the primary factor in explaining the ductility of various crystals including the initiation and propagation of cleavage crack.

This idea may really be applicable for the case of perfect crystals under homogeneous stress, which is idealized one of simple tension test of whiskers, or that superposed by hydrostatic tension, as discussed in the present paper. But actual problems yet remain in the criterions in atomistic regions with very sharp stress gradient on one hand, and relative importance of this factor compared with those of mobility and density of pre-existing dislocations on the other hand.

2) Propagation of cleavage crack is a particularly suitable theme for testing various theoretical predictions on these problems comparing with experiments, though our treatments remained rather crude because of many factors yet unknown. But we may note here some points for the purpose of critical discussions.

The first one concerns with the possibility of nucleation of dislocation loop at the tip of crack. According to Friedel's estimation[2] this process is considered to be a very easy one, because its activation energy is negative or very small at most as shown in his estimation, contrary to the conclusion of himself and also the assumption used by Tetelman.[3] The value of activation energy, however, become larger when we take into account more realistic factors as realistic elastic stress system and choice of the system of slip at the tip of crack which were treated by Tetelman. Furthermore, when we take into account non-linear compornents of strain at high stress level, for instance in the case of $\tau_{max}\simeq\tau_{th}$ the constraint factor $\sigma_{max}/\tau_{max} = 1/\alpha$ near the tip of crack is considered to be larger than that expected from linear elastic calculations, presumably rather resembles to the case of rigid-plastic or elastic-plastic stress system[22] in which the value of σ_{max}/τ_{max} was calculated as the order of $\simeq 5$ compared with that of $\simeq 1$ in simple dislocation model of crack tip. This factor may reduce a larger value of the activation energy. For instance, if we estimate $\sigma_{th}\simeq E/10$, $\tau_{th}\simeq G/30$ and $E/G\simeq 2$, then we obtain $1/\beta = \sigma_{th}/\tau_{th}\simeq 6$. On the other hand, if we take the probable value of the activation energy $k_s\tau_{th}$ in eq. (3) as 1.14 eV from the previous estimation, Fig. 6 and eq. (1), and that of $k_s\sigma_{th}(\beta-\alpha) = k_s\tau_{th}(1-\alpha/\beta) = 0.26$ eV in eq. (5) from the experimental value of Fe listed in Table 4, then we obtain $\alpha/\beta = 0.77$. This is the right order of magnitude expected from above considerations.

3) Then the second problem concerns with relative importance of the factor of nucleation of dislocation loop compared with those of pre-existing dislocations in the criterion of propagation of cleavage crack.

At first, when the ductility of crystal lattice is large, i.e. $(\beta-\alpha)$ or correspondingly the factor $k_s\sigma_{th}(\beta-\alpha)$ in eq. (5) is very small or negative, the tip of crack may be blunted by rather homogeneous nucleation of

dislocation loops before onset of nucleation of cleavage, even if the lattice resistance of dislocation is large and density of dislocation is very small, as illustrated in the case of Cu in Table 4. It might be the cases of many F.C.C. metals including their solid solutions.

And the second, if the velocity of the crack is sufficiently large, for instance larger than $C_t/10$ and nucleation of dislocations inhibited, then the multiplication of dislocations from pre-existing dislocations may not suffice to arrest the propagation of crack even if the lattice resistance is small and the density and the rate of multiplication is large as estimated by Tetelman[3] and also our theory.

This deduction seems to constracdict with the evidences of arresting temperature observed in iron and steels, which shows that fast propagating crack initiated in the region of low temperature is arrested at the region of higher temperature in the test of a plate with large breadth.[20]

Questions however may be remained for the role of grain boundary on this example, but we may point out that the plastic work at grain boundary might not be influenced so much by increasing temperature if we take into account only the factor of multiplication of pre-existing dislocations by the similar reasoning as in the case of tip of crack. Furthermore, our preliminary studies showed that the single crystals of pure iron which had very sharp notch yet showed finite transition temperature, and it was not so much influenced by pre-straining though the density of mobile dislocations was expected to be increased so much by this treatment. On the later account we may point out further that the lattice resistance of mobile dislocation in pure iron is considered to be much smaller than the stress required for unpinning.[17]

On the other hand, many twins usually observed on the surface of cleavage in iron, are considered to be nucleated at the tip of fast propagating crack,[17] because so many amount of deformation associated with the twins as observed may not be explained by only the mechanism of multiplication of pre-existing twinning dislocations.

And the other example is that the cleavability of single crystals of LiF (Harshaw) was little influenced by pre-straining of some percent in our preliminary experiment, though the density of mobile dislocations was increased to about $10^8/cm^2$ from the initial value of 10^5, or $10^2/cm^2$ for mobile ones as estimated by Tetelman. by the pre-straining. While it is expected that the plastic work in association with the propagation of crack would have been increased by the factor of 10^3 or 10^6 with the pre-straining according to Tetelman's theory.[3]

These evidences illustrated above seems to suggest that the ductility of crystals may be primarily related to that of perfect lattices, though the secondary effects of pre-existing dislocations may predominate in some cases. And the ductility of fast propagating crack, may provide critical case to test the above assumptions.

§ 6. Conclusion

Criterions for ductility of perfect lattice under homogeneous stress were presented in the forms that, the crystal may cleave or deform plastically as $\beta = \tau_{th}/\sigma_{th}$ is larger or smaller than $\alpha = \tau_{max}/\sigma_{max}$ at 0°K, while the ductitity depends on the relative magnitude of probabilities of nucleation of crack and dislocation loop at finite temperatures. The activation energies of nucleation of crack and dislocation loop were then calculated based on Peierls' approximation, and it was shown that these gave much smaller values than those predicted in previous theories. The theory was then applied for the problem of plastic work in association with the propagation of cleavage

crack, and it was shown that contribution of nucleation of dislocation loop at the tip of crack on the plastic work may predominate in the range where the velocity of crack and also temperature is sufficiently high compared with those due to multiplication of dislocations from pre-existing dislocations.

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Table /

$(\sigma_{yh}-\sigma_{\infty})/\sigma_{th}$	.01	.04	.1	.2
U_3 eV a=a	.134	.268	.424	.599
a=a/2	.017	.033	.053	.075

Table 1. Numerical examples of U_c calculated by the equation (1), where $E = 2\times10^{12}$, $\nu = 0.25$, $\gamma = 1.2\times10^3$, $a = 2.86\times10^{-8}$ C.G.S. (Fe).

Table 2

F.C.C. $(\bar{1}11)$ [211]

$\frac{\tau_{th}-\tau}{\tau_{th}}$	.01	.04	.1	.2
$U_3(P)$ eV	.0098	.0195	.031	.0436
$U_3(C)$	.0585	.234	.538	1.17

B.C.C. $(11\bar{2})$ [111]

$\frac{\tau_{th}-\tau}{\tau_{th}}$	.01	.04	.1	.2
$U_3(P)$ eV	.0138	.0276	.0436	.0617
$U_3(C)$	.0538	.215	.538	1.08

$G = 8 \times 10^{11}$, $\nu = 0.25$, $a = 2.86 \times 10^{-8}$ C.G.S.

Table 2. Comparisons of U_s between Cottrell's theory $U_3(c)$ and Peierls' approximation $U_3(p)$. For F.C.C. we assumed $\lambda = a/2\sqrt{6}$, where a is lattice constant, correspondingly $G/\tau_{th} = 17.8$ in Peierls' approximation. On the other hand, we took $\lambda = b$ and same value of $G/\tau_0 = 17.8$ in Cottrell's formula cited in Fig. 6 for the sake of comparison. For B.C.C. we took $\lambda = a\sqrt{3}/6$, corespondingly $G/\tau_{th} = 8.9$ in Peierls' approximation, and same value of G/τ_0 in Cottrell's formula.

Table 3

	$\frac{\tau_{max}}{\tau_p}$	$A(eV)$	$\frac{2C_t}{V_0}$
LiF	4~10~40	0.2	~2 (600°K) 2×10^2 (300 ") $>2\times10^5$ (77 ")
Fe	100~1000	0.1	~2 (300°K)
Cu	$10^{\frac{4\sim5}{}}$	0.05	

Table 3. Experimental values taken from literatures. The underlined values were used in the calculations of Table 4.

Table 4

		left	right 1st	2nd	4th	5th
LiF	1200°K	2.8	3	2. ×0.3	0.3	− 1.1
	600°K	1.4	3	1. ×0.3	0.3	− 2.2
	300°K	2.	3	0.5×2.3	2.3	− 4.4
	77°K			0.1×5.3	>5.3	− 17.1
Fe	600°K	4.6	6	2.0×0.3	0.3	− 2.3
	300°K	2.	6	1.0×0.3	0.3	− 4.6
	90°K			0.3×1.		− 15.3
Cu	90°K	10.5	12	0.5×0.3	0.3	− 2.0
	4°K					− 45.0

Table 4. Estimated values for the terms in the equation (5).

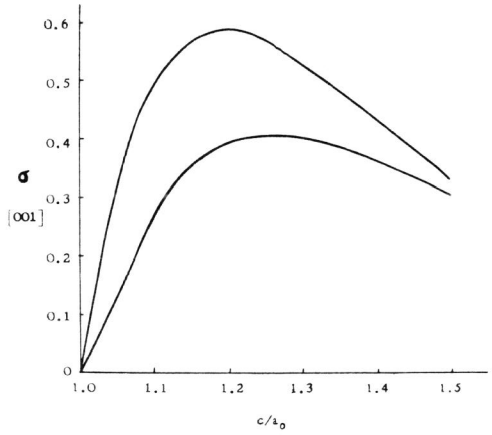

Fig. 1 Tensile stress-strain relations of Lennard-Jones type crystal n = 12, m = 6, n; exponent of repulsive potential, m; that of attractive potential, C; lattice constant parallel to tensile axis, a_0 ; lattice constant of stress free crystal. Upper curve is the case where lateral strain is restricted, and lower curve free from constraint. The curves were calculated by electronic computer.

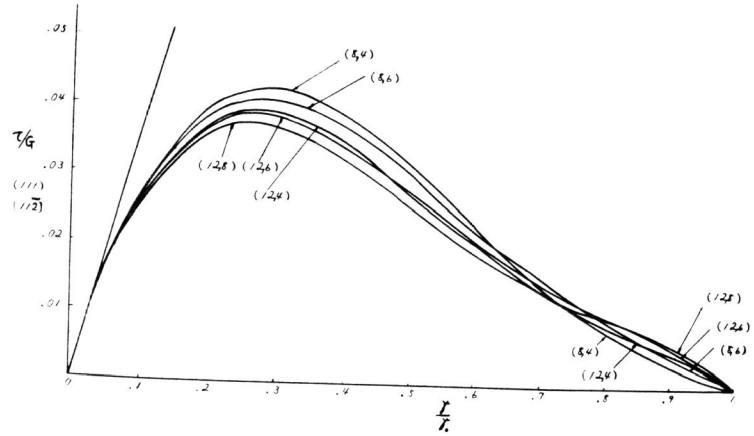

Fig. 2 Shearing stress-strain relations of Lennard-Jones type crystals with various exponents of potentials (n,m). Shear is applied in the direction $[11\bar{2}]$ on the plane (111), where the strain in $[1\bar{1}0]$ is restricted and the normal stresses in [111] and $[11\bar{2}]$ are free. The curves were fittet by appropriate quadruple equations so as to coincide with the calculated values of elastic constants at initial states and also the elastic constants and potentials at the maximum potential states. And E/G= 3.2126 when n= 12 and m= 6, where E= E [100] constraint free, G= G (111) $[11\bar{2}]$ strain in $[1\bar{1}0]$ is restricted.

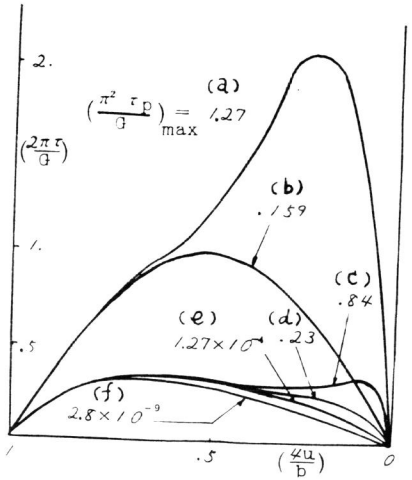

Fig. 3 Dependency of Peierls' stress on various form of shearing stress-strain relations of crystal lattices calculated based on generalized Peierls' approximation. Curve (b) is Peierls-Nabarro's case, and curve (f) is Foreman Jaswon and Wood's case.

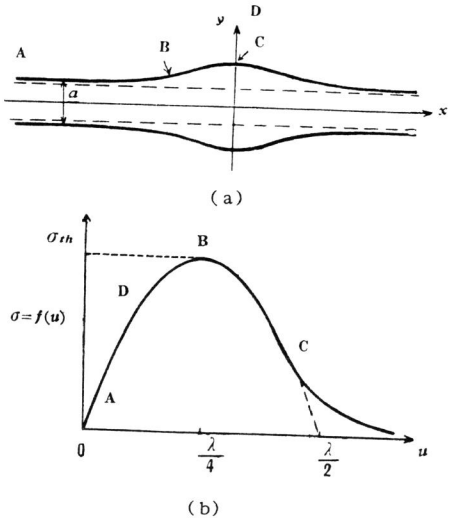

Fig. 4a, b. Model of nucleus of crack.

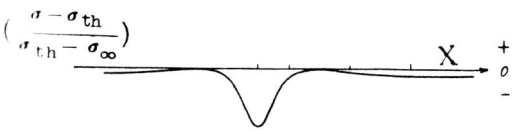

Fig. 4C Stress distribution along the axis χ when $(\sigma_{th} - \sigma_\infty)/\sigma_{th} \ll 1$

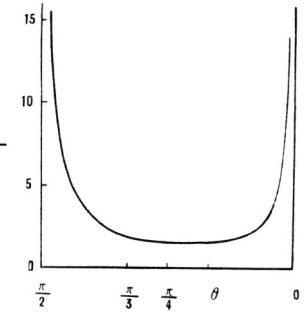

Fig. 4d Dependency of size of nucleus of crack $2\chi_c$ on the applied stress σ_∞. χ_c is the length BC in Fig. 4a, $\sin\theta = \sigma_\infty/\sigma_{th}$ $\chi_c \to \infty$ as $\sigma_\infty \to \sigma_{th}$, the curve is applied only for $\theta \geq \pi/3$.

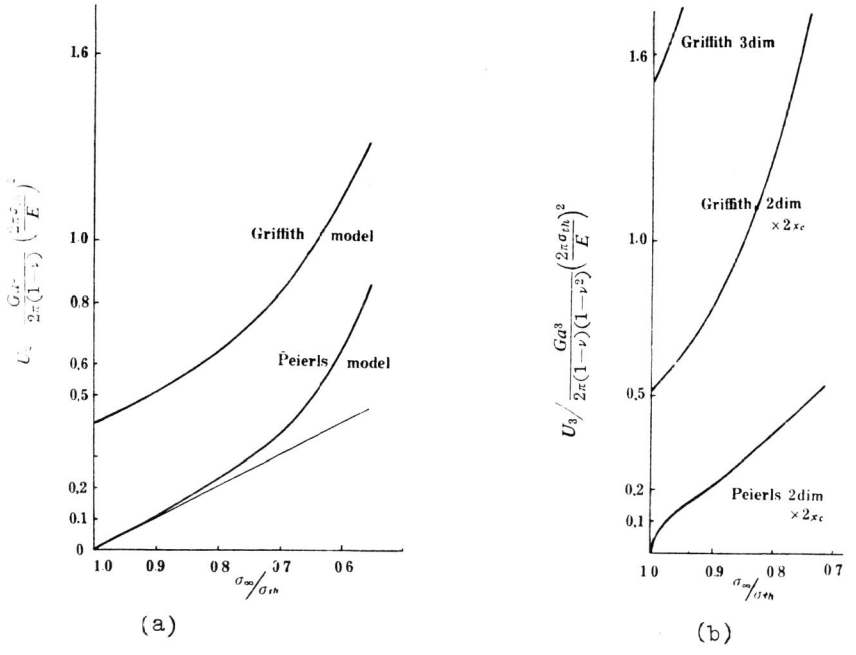

Fig. 5a, b Activation energies of nucleation of crack calculated by Griffith's theory and Peierls' approximation, a; two dimentional case, b; three dimentional case, where U_c is assumed to be equal to $2\chi_c U_{c,2}$. It is noted that Griffith's theory predict non-zero activation energy at $\sigma = \sigma_{th} = \sqrt{Er/a}$.

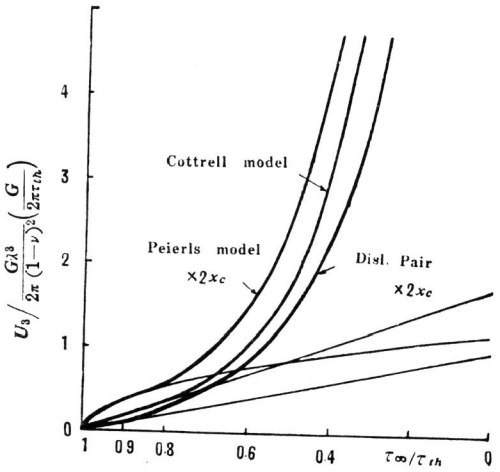

Fig. 6 Activation energies of nucleation of dislocation loop calculated by Cottrell's theory and Peierls' approximation, where $U_S = 2\chi_c U_{S,2}$. Cottrell's equation can be written in the form when $\tau/\tau_0 \simeq 1$,

$$U_s = \frac{1}{2} G b^3 \left(\frac{G}{2\pi\tau_0}\right)\left(1-\frac{\tau}{\tau_0}\right),$$

where b is magnitude of Burgers vector, τ_0 a constant related to the energy of dislocation and not equal to τ_{th} in general, but we put $\lambda = b$ and $\tau_0 = \tau_{th}$ for convenience's sake in this figure. While $\lambda = 2\pi b \times \tau_{th}/G$ in Peierls' approximation.

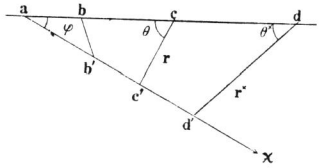

Fig. 7 Spreading of dislocation loop nucleated at the tip of crack. Dislocation loop nucleated at the point a spreads to the points b', c' and d' on the slip plane ax, according as the tip of crack proceeds to the points b, c and d. In the evaluation of q, we estimated the diameter of spreading of a loop by the distance ad' assuming that the velocity of dislocation was retarded to V/2 at the point d', and $\varphi \simeq \theta' \simeq 45^\circ$ and consequently $K \simeq \frac{1}{2}$.