INFLUENCE OF CRACK TIP SHIELDING ON SILICON TOUGHNESS THEORETICAL AND EXPERIMENTAL STUDY

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A theoretical model for plastic relaxation at a crack tip, including a dislocation free-zone is proposed. The characteristics of the plastic zone deduced from this model are of the correct order of magnitude compared to those obtained on relaxed crack in Silicon.

INTRODUCTION

The first part of this paper is concerned with a theoretical study of dislocation distribution ahead of a crack tip with special attention paid to the influence of the plastic zone on the material toughness. The problem has been solved using the K concept in order to avoid accounting for the specific geometry of the crack and the loading. The results are then compared to previous models (1,2) in which the crack is represented by a continuous distribution of dislocations. The second part of the paper deals with the application of our model to the case of Silicon for which an important amount of experimental results is available, from X-Ray Topography observations (3 to 6), etch pits counts (6), and mechanical tests (7 to 9).

EQUILIBRIUM CONFIGURATION OF DISLOCATIONS

The stress intensity factor for a semi-infinite crack loaded under antiplane conditions (mode III) is given by K. We have assumed that the crack plane lies parallel to a slip plane of the solid and the

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crack tip is parallel to a glide direction in this plane. The infinite material is characterized by a shear modulus μ and a friction stress τ_y. For sufficiently high values of K (2,5) a set of straight parallel screw dislocations is emitted (from either the crack tip or bulk sources) in the slip plane considered above and move until the stress acting on them equal zero.

Basic Equations

This last condition is expressed by the equilibrium equation :

$$\frac{K}{\sqrt{2\pi X}} - \frac{\mu b}{4\pi X} + \frac{\mu}{2\pi}\int_{A_1}^{A_2} \sqrt{\frac{Y}{X}}\,\frac{\rho(Y)dY}{X - Y} - \tau_y = 0 \quad \text{.................. (1)}$$

The first term corresponds to the external stress acting on a dislocation located at the distance X from the crack tip (Fig.1), the second to the image force (10,11), the third to the interaction with the other dislocations of the plastic zone. It must be pointed out that the usual interaction law between dislocations is modified by the proximity of free surfaces, as was shown by the conformal mapping method (10) or by the image dislocation distribution method (11). The number N of dislocations extending form the abscissa A_1 to A_2 is related to the distribution function :

$$Nb = \int_{A_1}^{A_2} \rho(X)\, dX \quad \text{.............................. (2)}$$

Equation (1) is an integral equation (12). After multiplying by $\sqrt{X}$, a previously solved equation is obtained (13), whose solution is given by :

$$\rho(Y) = -\frac{1}{\pi^2}\sqrt{\frac{(A_2-Y)(Y-A_1)}{Y}} \int_{A_1}^{A_2} \frac{\Omega(X)\, dX}{(X-Y)\sqrt{(A_2-X)(X-A_1)}} \quad \text{.... (3)}$$

with $\Omega(X) = \frac{2\pi}{\mu}\sqrt{X}\left(\frac{K}{\sqrt{2\pi X}} - \frac{\mu b}{4\pi X} - \tau_y\right)$

The solution (equation (3)) exists when the following condition is fulfilled :

$$\int_{A_1}^{A_2} \frac{\Omega(X)\, dX}{\sqrt{(A_2-X)(X-A_1)}} = 0 \quad \text{.................... (4)}$$

Shielding Effect

Since a crack exerts a force on a dislocation (image force), the laws of mechanics imply that the dislocation must exert an equal and opposite force on the crack. This effect, the so-called shielding effect (10), leads to a decrease ΔK of the stress intensity factor from K to an effective value K_e :

$$K_e = K - \frac{\mu}{\sqrt{2\pi}} \int_{A_1}^{A_2} \frac{\rho(Y)dY}{\sqrt{Y}} = K - |\Delta K| \qquad (5)$$

while the crack extension force $\frac{K^2}{2\mu}$ decrease to $\frac{K_e^2}{2\mu}$.

Solutions

With the introduction of dimensionless parameters, $a = A/A_o$, $k = \pi K/K_o$ and $p^2 = 1-A_1/A_2$, equation (4) leads to the following relation after some integral calculations (14) :

$$k = E(p)\ \sqrt{a_2} + K(p)/\sqrt{a_2} \qquad (6)$$

The complete elliptical integrals of first and second kind, K(p) and E(p), can be calculated accurately by polynomial approximations (15). The combination of equations (3) and (5) leads to :

$$k_e = K(p)\ \sqrt{a_1} + E(p)/\sqrt{a_1} \qquad (7)$$

The number of dislocations can be derived either by inserting relation (3) in equation (2) or by general considerations. The second method (16) postulates that the decrease in the crack extension force due to N dislocations is equal to the force exerted by the crack on a superdislocation of Burgers vector Nb. The equilibrium of the superdislocation is reached when this force is counterbalanced by the friction stress :

$$\frac{K^2}{2\mu} - \frac{K_e^2}{2\mu} = N\ \tau_y\ b \qquad \text{or} \qquad k^2 - k_e^2 = N\ \pi^2 \qquad (8)$$

It is noteworthy that the knowledge of the distribution function is no longer necessary.

The effective stress intensity factor k_e has been plotted as a function of k for several values of the free parameters a_1, a_2 (Fig.2) and N (Fig.3). The possible solutions in the (k_e, k) plane are limited by two curves. The upper curve ($k_e = k$) corresponds to the brittle case (no plastic relaxation), the lower curve to the minimum possible value of k_e,i.e to maximum shielding. Points under this last curve represent distributions of dislocation with positive and negative signs. Because only positive sign dislocations obey equation (1) these solutions have no physical sense. A minimum value, $K_o = \sqrt{2\mu b \tau_y}$ of K, is necessary to overcome the image stress on the first dislocation. It can be verified from equation (1) that an unstable equilibrium position $A_o = \mu b/4\pi\ \tau_y$ corresponds to this value.

Comparison with previous models

The original BCS Model (1) of a totally relaxed ($K_e = 0$, $A_1 = 0$) embedded crack (length 2C, uniform loading σ) has been generalized by Chang and Ohr (2) who introduced a dislocation-free zone (DFZ) (Fig.4). The fact that $A_1>0$ prevents the crack from relaxing completely. The corresponding results can be related to our results only for the limit case when there is no interaction between the two plastic zones of the embedded crack, i.e. when A_2 is much smaller than C. In these conditions the K value for a semi-infinite crack would be related to the uniform loading stress σ of BCS model by the relation $K = \sigma\sqrt{2\pi c}$ (11).

For A_2 much smaller than C, equations (25) and (32) of Chang and Ohr's paper tend to the first term of equation (6) and to the first term of equation (7), respectively. The missing terms arise from the image term of equation (1) i.e. $\mu b/4\pi X$. To explain these discrepancies we shall follow Li's arguments (11) : an image dislocation distribution $\rho_q^i(Y)$ inside the fictitious crack is associated with the q^{th} dislocation of the N dislocations of the plastic zone (Fig.4). To account for the crack loading a distribution $\rho^{ex}(Y)$ is added inside the crack. The q^{th} dislocation is submitted to the interaction with the (N-1) image distributions $\rho_r^i(Y)$ with $r\neq q$, to its own image distribution $\rho_q^i(Y)$, (giving rise to a stress $-\mu b/4\pi Y_q$) to the (N-1) dislocations of the plastic zone, to the external stress and finally to the friction stress. In BCS formulation these last two terms, summarized under the label $\Omega(Y)$ are related to the interaction terms by the following equation :

$$\Omega(Y_q) = \frac{\mu}{2\pi}\int_D \frac{\rho(Y)dY}{Y-Y_q} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (9)$$

which means that the stress in Y_q is equal to zero. The action of the dislocation located in Y_q is not taken into account (for this reason the principal value of the integral is assumed) and the corresponding image distribution $\rho_q^i(Y)$ is also removed. Thus Chang and Ohr's model (or BCS model), corresponding to a configuration of (N-1) dislocations near a crack, including the $\rho_r^i(Y)$ image terms ($r\neq q$). However it fails to represent an N dislocations pile-up because the interaction between the dislocation in Y_q and its image distribution $\rho_q^i(Y)$ is omitted.

N.B. : When multiplied by $\sqrt{2\pi X}$, the limit value of equation (1) for vanishing X, gives :

$$K - \lim_{X\to 0}\left(\frac{\mu b}{4\pi X}\right) - |\Delta K| = 0 \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (10)$$

Obviously this condition is achieved when the second term is omitted, leading to the BCS condition, i.e. total relaxation with a vanishing DFZ.

APPLICATION TO SILICON

For three unknowns k_e, a_1 and a_2 only two equations ((6) and (7)) are available. The third relation, needed for a complete solution of the problem, has been obtained experimentally.

Experimental procedure

A totally brittle {111} cleavage is introduced at 20°C in a dislocation free floated-zone Silicon single crystal (3,5,7). This pre-cleaved sample is then loaded under constant P at a temperature high enough for silicon to be ductile (T>650°C). This load is related to the mode I applied stress intensity factor K_I by a calibration function f depending on the crack geometry and loading conditions, $K_I = P \times f$. The loading time has been chosen long enough for the plastic zone ahead of the crack tip to saturate. This last point has been checked by in-situ X-ray topography (4) asserting an equilibrium configuration of the dislocations of the plastic zone. Then the dislocation pattern has been frozen in by cooling down to 20°C where dislocation mobility is negligible.

K_e determination

For our specimen geometry it has been shown that blunting is negligible relative to shielding (8,9) in Silicon. Thus the high temperature equilibrium stress intensity factor is given by equation (5). After freezing-in of the dislocations the stress intensity factor at room temperature K^{RT} is related to the applied load P^{RT} by the relation :

$$K_I^{RT} = P^{RT} \times f - |\Delta K_I| \quad \text{.................................(11)}$$

Fracture occurs under a load P_C^{RT} for $K_I^{RT} = K_{IC}$, because the crack is assumed to remain sharp after pre-straining. The K_{Ie} values are deduced from :

$$K_{IC} = P_C^{RT} \times f + K_{Ie} - K_I \quad \text{.................................(12)}$$

Discussion

In our experiments under mode I crack opening, dislocation loops develop around the intersection of the crack tip with essentially two glide plane families, giving rise to four extending lobes (3,4,7), i.e. to a three dimensional plastic zone. The first difficulty in solving such a problem is to introduce the interactions between dislocations of distinct lobes. The second one is to calculate the shielding effect of dislocation loops of any orientations ; in fact, results are available only for straight dislocations (17).

The stress near a crack corresponds to the sum of a singular term proportionnal to $K/\sqrt{r}$ and to a non-singular term depending on the loading and sample geometries. Only the first one is involved in our model, so the small scale yielding hypothesis is assumed, limiting the accuracy of the conclusions. In particular, in silicon, it has been shown that the second term can influence the extension of the plastic zone (6).

From previous remarks it results that only a rough comparison is possible between our experimental and theoretical observations. We have calculated the characteristics of a mode III plastic zone (A_1, A_2, N) giving the same shielding as our experiment, and compared with mode I plastic zone characteristics. These last features, obtained on five samples by etch pits counts and fracture tests, have been summarized in Table 1.

TABLE 1 - Mode I Experimental Results

SAMPLE	K_I (MPa$\sqrt{m}$)	K_{Ie} (MPa$\sqrt{m}$)	A_2 (mm)	N (by lobe)
F22	0.55	0.068	1.45	468
F14	0.66	0.186	1.45	796
F17	0.66	0.037	2.15	830
F36	0.77	0.168	2.75	2 900
F23	0,77	0.300	2.85	3 050

TABLE 2 - Calculated Values for τ_y = 6 MPa

SAMPLE	K_I (MPa$\sqrt{m}$)	A_1 (µm)	A_2 (mm)	N
F22	0.55	1.74	3.29	866
F14	0.66	22.8	4.66	1 165
F17	0.66	0.22	4.74	1 264
F36	0.77	15.8	6.40	1 642
F23	0.77	75.5	6.23	1 455

Different values of τ_y are chosen to relate the dimensionless coordinates k, k_e (Fig.2) to the experimental values K and K_e. A reasonnable fit is obtained for τ_y = 6 MPa, a value which is of the same order of magnitude as the experimental starting stress for dislocation movement in silicon (∿ 3 MPa (18)), the excess being attributed to the interactions between dislocations of different glide planes. For a given load, A_2, and N variations are closed to τ_y^{-2} and τ_y^{-1}, respectively like in BCS model. Calculated values of A_1 and N are listed in Table 2.

Comparisons between tables 1 and 2 show that the calculated values of A_2 and N have the correct order of magnitude. No DFZ has been observed by X-Ray topography or etch pit methods, perhaps because of the low resolution of the techniques ; calculated values are not far from the resolution limits (except for sample F23).

CONCLUSIONS

Our model allows an estimate of the characteristics of the plastic zone at the tip of a mode I crack, only when a complementary experimental relation is available. The stress intensity factor at equilibrium K_e, determined by fracture experiments, must be related to a physical property of the material. Particularly, it must depend on the degree of stress relaxation at the crack tip, thus on the ability of the crack to create enough dislocations to lower the K_e value or the DFZ length. For example, the physical parameter could be the critical stress (or stress intensity factor) (5) for dislocation generation at or near the crack tip.

SYMBOLS USED

$K_o = \sqrt{2\mu b \tau_y}$ (MPa$\sqrt{m}$), $A_o = \mu b/4\pi\tau_y$ (m)

K = Applied stress intensity factor (reduced value : k)

K_e = Effective stress intensity factor (reduced value : k_e)

$K(p) = \int_0^{\pi/2} d\theta \sqrt{1-p^2\sin^2\theta}$ = Elliptical integral of first kind

$E(p) = \int_0^{\pi/2} d\theta / \sqrt{1-p^2\sin^2\theta}$ = Elliptical integral of second kind.

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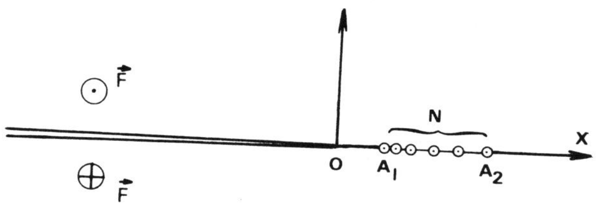

Figure 1 : Sketch of the crack and its associated yielded zone

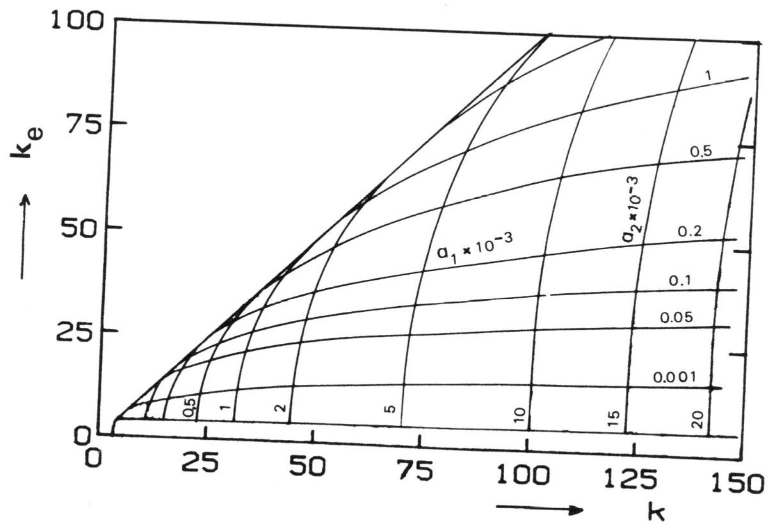

Figure 2 : Variations of k_e versus k for different a_1 and a_2 values

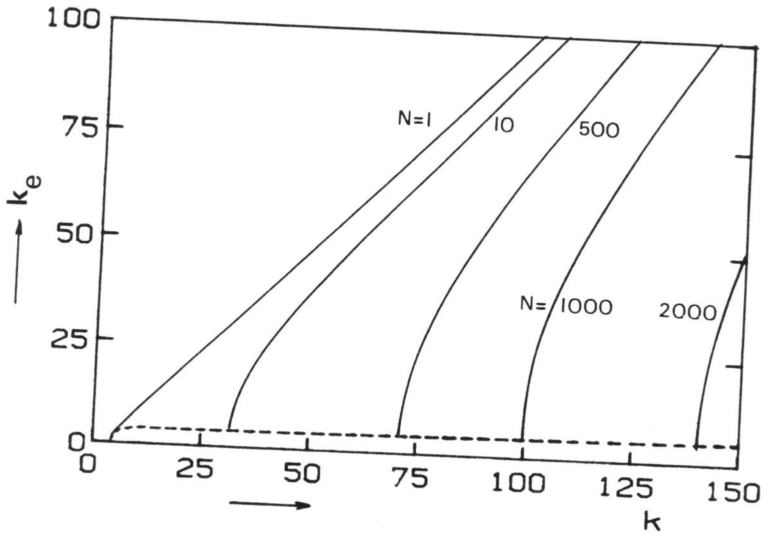

Figure 3 : Variations of k_e versus k for different N values

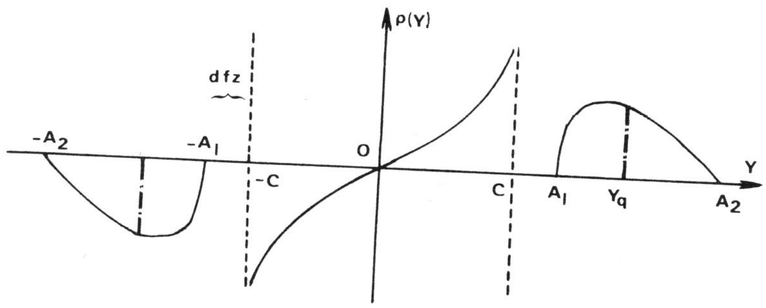

Figure 4 : Distribution of dislocations modelling a relaxed crack (see ref.(2))