A New Look at Cleavage Crack Formation in Semi Brittle Materials

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Abstract. The formation of sessile cleavage crack nuclei of the type $a\langle \mathbf{001} \rangle$ from glissile dislocations of the type $\frac{a}{2}\langle \mathbf{111} \rangle$ in BCC materials is considered. It is shown that an energy reduction is not a sufficient criterion to predict formation of crack nuclei; interaction forces must be considered as well. The tendency to form cleavage crack nuclei in BCC crystals is explained by the fact that glide dislocations are inevitably driven into stable configurations for the formation of microcrack nuclei. It is further shown that the conditions for microcrack growth are far more restrictive. A general framework for analyzing dislocation interactions using closed-form solutions is outlined.

Introduction

In real materials, dislocations may be considered, as a first approximation, to be randomly distributed. However most models for dislocation reactions *assume* a convenient symmetry and typically consider the energy reduction that occurs when these dislocations come together to react. It is generally assumed that the reaction is favoured if there is an energy reduction. For example, Cottrell [1] considered two parallel dislocations lying on intersecting $\{110\}$-type planes in a BCC material as shown in Fig. 1.

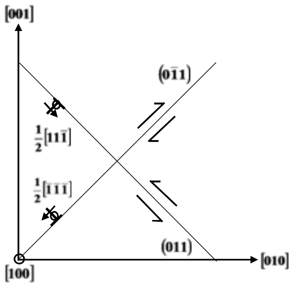

Fig. 1. Dislocations, relative to crystallographic axes. The slip planes are viewed edge on. Shear stresses are shown for an equivalent applied tensile stress along [001]. The Burgers vectors are foreshortened in this view.

A cleavage crack nucleus is formed by the combination of these two dislocations:

$$\frac{a}{2}[\mathbf{11\bar{1}}]+\frac{a}{2}[\mathbf{\bar{1}\bar{1}\bar{1}}]\rightarrow a[\mathbf{00\bar{1}}] \tag{1}$$

The change in energy (reduction) for an isotropic material is:

$$\Delta E_{el} = -\frac{Ga^2}{4} \tag{2}$$

A microcrack nucleus consisting of two sessile dislocations is shown in Fig. 3.

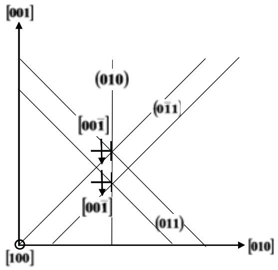

Fig. 2. Formation of sessile edge dislocations on (010) plane. Each dislocation results from the combination of two glide dislocations shown in Fig. 1.

However, additional factors must be considered in assessing the formation of a cleavage crack:

1. Interactions between the first two dislocations that form the original sessile dislocation that have no a priori assumptions about symmetry.
2. Interactions between the sessile dislocation and the formation of an adjacent sessile by glissile dislocations.
3. The interaction between the sessile dislocations and the formation of subsequent sessile dislocations.
4. A thermodynamic criterion for microcrack stability and extension.
5. Effects of anisotropy.

In this report, questions 1-3 are addressed are addressed with no a priori geometric assumptions using a computational framework developed by the authors. Questions 4-5 are currently under investigation. Subsequent sections of the paper are organized as follows:

- Description of a generalized computational framework for two dislocation interactions.
- Application of methodology to the problem of interactions between two dislocations to determine the angular domain under which there are attractive junctions (i.e. easy formation of cleavage crack nuclei).
- Extension of model to interactions of sessile and glissile dislocations and the growth of microcracks.
- Conclusions and comparison with previous results.

Computational Framework for Glissile Dislocation Interactions

Overview. In carrying out calculations that involve interactions between parallel dislocations of arbitrary character (1 and 2 say), the stress field of 1 exerts a force on 2. If the dislocations are not on parallel slip planes the stress fields must be appropriately expressed in the correct frame of reference in order to be able to use conventional force equations. Since the calculations relate to attractive and repulsive glide forces, great care must be exercised in ensuring that all of the signs and conventions are self consistent. The various steps in calculating the glide force interactions are summarized below.

Development of Coordinate Systems. To begin the calculation, each dislocation is placed in its own Cartesian coordinate system. The coordinate systems for dislocations 1 and 2 are shown in Fig. 3.

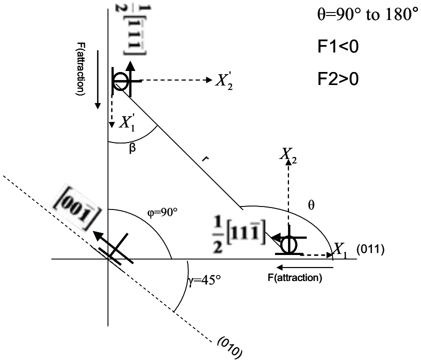

Fig. 3. Definition of coordinate systems for dislocations 1 (unprimed) and 2 (primed). In addition the force requirements for attractive interaction in the quadrant pictured are indicated relative to the axis systems.

Dislocation 1 is on the horizontal slip plane and its axis system is denoted by X_1, X_2. The coordinate system for dislocation 2, whose slip plane has at least a vertical component, is denoted by X_1', X_2'. A fully consistent coordinate system may be developed in terms of the slip plane, Burgers vector and common positive direction using vector calculus. Positive unit vectors parallel to the coordinate axes for the first dislocation are then denoted $(\vec{\mathbf{x}}_1, \vec{\mathbf{x}}_2, \vec{\mathbf{x}}_3)$. Positive unit vectors parallel to the coordinate axes for the second dislocation are defined in an analogous manner with the axes being denoted by primes, i.e. $(\vec{\mathbf{x}}_1', \vec{\mathbf{x}}_2', \vec{\mathbf{x}}_3')$. Note that $\vec{\mathbf{x}}_3 \equiv \vec{\mathbf{x}}'_3$ (i.e. the positive sense for both dislocations is the same).

Calculation of Attractive/Repulsive Junctions. Having defined a coordinate system for both dislocations, the normalized glide force on each dislocation (i.e. $Force \Big/ \left(\frac{Ga}{2\pi r}\right)$) may be calculated for each dislocation as a function of orientation. In carrying out this calculation it is *extremely important* to respect all sign conventions so that the correct algebraic sign for the force on each dislocation is obtained. This is absolutely critical in determining simultaneous signs of the force on each dislocation and hence whether or not the junction is attractive or repulsive. This calculation is carried out in terms of the approach angle θ which has been defined in Fig. 2. The steps required to compute the force on dislocation 2 due to the stress field of dislocation 1are:

- Write down the stress fields for dislocation 1 in its own coordinate system for the edge and screw components as a function of θ.
- Using a tensor transformation, write down the stresses of the edge component of dislocation 1 in the coordinate system of dislocation 2. Note that the shear stress of interest is denoted σ_{12}'.
- Compute that component of the glide force on dislocation 2 due to the edge component of 1 by use of the equation:

$$F_{2e} = -b_{2e} \cdot \sigma_{12}' \tag{3}$$

- Compute the component of the glide force on 2 due to the screw component of 1. This may be simply done by decomposing the total screw/screw interaction force on 2 in the direction of the junction. The symmetry of the screw stress field makes tensor transformation an unnecessarily complicated step. The result of that calculation is:

$$F_{2s} == -b_{1s}b_{2s}\cos(\theta-\phi) \tag{4}$$

- The total normalized force on dislocation 2 due to the stress field of dislocation 1 is then the algebraic sum of the forces of (3) and (4):

$$F_{2t}(\theta) = F_{2e}(\theta) + F_{2s}(\theta) \tag{5}$$

The same procedure as described in the preceding section can be used to determine the total force on dislocation 1 due to dislocation 2. The interaction glide forces for both dislocations are shown in Fig. 4.

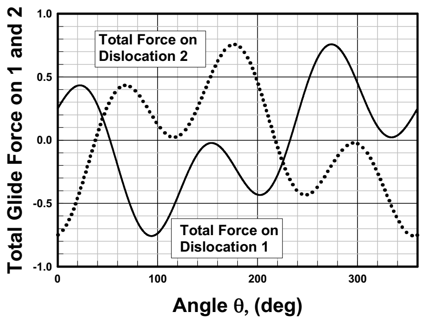

Fig. 4. Total glide force on dislocations 1 and 2. Note that the forces are given in the frame of reference of each individual dislocation. Regions of attraction are between arrows.

Computational Framework for Sessile/Glissile Dislocation Interactions

Overview. Given the fact that the nucleus of a microcrack forms quite readily, the next question to arise is how that nucleus can grow by a glide mechanism. In other words, what stresses must the glissile dislocations overcome to form another sessile dislocation on the slip plane next to the first sessile dislocation? The situation is shown in Fig. 5. A major question is what are the interactions between the sessile dislocation and the glissile dislocations as a function of the approach distance denoted r_{34} on the diagram? Obviously the further apart the two sessile dislocations, the less like a crack is this pile up. On the other hand, the closer together the sessile dislocations, the higher the interaction forces must have been to bring this situation about or the external forces must have been large enough to overcome repulsive dislocation interactions. To answer this question, calculations similar in concept but considerably more complex, were carried out. Selected results are shown in Fig. 6 for various values of r_{34} and a fixed value of r. It is clear that the results depend sensitively on the approach distance. The angular values for stable and metastable configurations were also examined and results are shown in Table 1; the terms "stable" and "metastable" will be defined later.

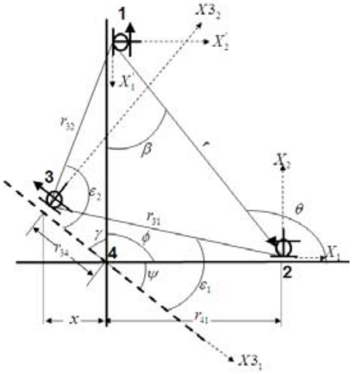

Fig. 5. Representation of the angles and distances that define the configuration where a series of sessile dislocations can be formed. The bold numbers 1-4 are used to describe individual glissile and sessile dislocations.

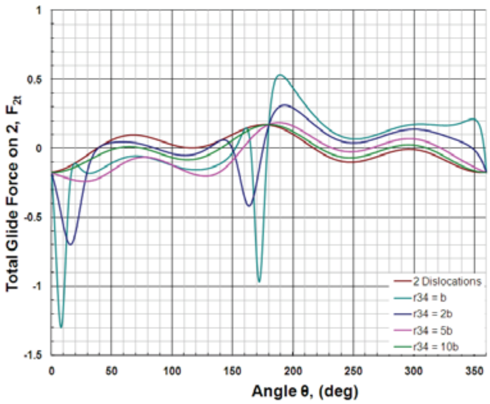

Fig. 6. Glide force on dislocation 2 for several values of r_{34} and r=5$|\mathbf{b}_1|$.

Table 1. Stable and metastable configurations for $r = 5$ and various values of r_{34}. 'S' denotes a stable configuration, 'M' denotes a metastable configuration, 'A' denotes an attractive configuration, and 'R' denotes a repulsive configuration.

r_{34} (nxb_3)	Stable/Metastable values of θ			
1	45 (S,R)	93.7 (M,R)	166.2 (S,R)	178 (M,R)
	225 (S,R)	272 (M,R)	283.8 (S,R)	356.3 (M,R)
2	45 (S,A)	110.5 (M,R)	154.4 (S,R)	172.9 (M,R)
	225 (S,R)	277.1 (M,R)	295.6 (S,R)	339.5 (M,R)
5	45 (S,R)	151.4 (M,R)	225 (S,R)	298.6 (M,R)
10	45 (S,R)	139.1 (M,R)	225 (S,A)	310.9 (M,R)
20	45 (S,A)	135.6 (M,A)	225 (S,A)	314.4 (M,A)
40	45 (S,A)	135 (M,A)	225 (S,A)	315 (M,A)
Infinity	45 (S,A)	135 (M,A)	225 (S,A)	315 (M,A)

Discussion of Results

Glissile Dislocations and Microcrack Nucleus. In the preceding paragraphs, a generalized argument has been made that establishes the dislocation orientations where the forces on the dislocations are directed to a common junction. However, this in itself is not sufficient to say whether or not the junction is attractive or repulsive. The relative magnitude of the glide forces acting on each dislocation, which can influence whether the dislocations are "pushed" in or out of attractive or repulsive regions, must be considered along with the stability of given configurations since this will change θ. In essence, the question is whether there are configurations where the relative magnitudes on each dislocation does not change as they move towards or away from the common junction. These configurations are labeled here as "stable" and they can be attractive or repulsive; a "metastable" configuration occurs when the magnitude of the force on each dislocation is equal at a given orientation, but the signs of the forces on the dislocations at larger or smaller angles moves the dislocations away from these special configurations. As an example of a stable configuration, consider an angle between dislocations 1 and 2 of 134˚. In this configuration, the force on each dislocation is moving it to the common junction; however, the relative magnitude of the force of dislocation 1 is greater than that of dislocation 2 as seen in Fig. 4. Thus, dislocation 1 will move further on its slip system than dislocation 2 and the angle between them will decrease. As the angle continues to decrease, the magnitude of the force on 1 is always greater than the force on 2 (causing the angle to further decrease) until about 70^o at which point the forces are balanced. At this point the force on 1 is directed away from the junction and the force on 2 is directed towards the junction. This means that the angle will continue to decrease. As the angle decreases, the force on 2 away from the junction is less than the force on 1 towards the junction which means that the angle decreases. When it reaches about 52^o the force on 1 is zero and the force on 2 is towards the junction. Thus, the angle will still decrease. When the angle is less than 52^o but greater than 45^o, both dislocations experience forces towards the junction with the force on 2 always being larger than the force on 1. This means that the angle will decrease and a particularly stable configuration results at 45^o; both dislocations experience equal forces towards the junction. Any movement away from this symmetry point by either dislocation will result in forces that tend to restore the 45^o configuration. Similarly, if one dislocation moves to make the angle less than 45^o there are forces that restore the 45^o configuration. For example, suppose that somehow the dislocations move to make a 40^o angle. The force on 2 is negligible and the force on 1 is directed towards the junction, which will restore the 45^o configuration. When θ equals 45˚, the magnitude of the force on each of them is equal, and they approach the common junction at an equal rate. Thus, the two dislocations will move to form the sessile dislocation at the common junction only when the magnitude of the force acting on them is equal and pushes them both towards the junction. One can make similar arguments for any relative orientation that is chosen leading to the conclusion that all that is required to nucleate a microcrack nucleus is a stress high enough to move dislocations to a point where the interaction forces pull the dislocations to the common junction. In short, in this model, cleavage occurs at a stress just above the lattice friction stress in agreement with Cottrell [1] and with more recent work of Li and Yao [2]. These calculations demonstrate why plastically-induced cleavage crack formation is so frequently seen in BCC materials; all configurations reach the symmetrical and stable configuration for microcrack formation (Table I). Another factor in cleavage is the ratio of the cleavage stress to the lattice friction stress. If the lattice friction stress is high, then the dislocations making up the crack nucleus will not move on their slip plane, allowing stresses to build up in front of the microcrack that will eventually cause cleavage. The friction stress on {001} planes in BCC is much higher than the friction stress on {001} planes in FCC (potential cleavage planes) so cleavage is much more probable in BCC structures even though there are more slip systems in BCC.

Growth of Microcrack Nucleus. Figure 6 shows that there is great sensitivity of the glide force on dislocation 2 as a function of the presumed distance between the two sessile dislocations. Stable and metastable configurations for r = 5 $|\mathbf{b}_1|$ and r_{34} equal to various integer multiples of $|\mathbf{b}_3|$ are shown in Table 1. When r_{34} is equal to $1|\mathbf{b}_3|$, there are no regions where the dislocations are attracted to the common junction. Thus, in the absence of an external force, the glissile dislocations will always be repulsed from the sessile dislocation. This would imply that the notion of having edge dislocations immediately adjacent to one another in the absence of an external force is an unattainable idealization. There are stable configurations when angle between the dislocations is 45˚, 166.2˚, 225˚, and 283.8˚. For these angles, the dislocations will move away from the common junction at an equal rate. There are also metastable configurations at θ equal to 93.7˚, 178˚, 272˚, and 356.3˚. There is a similar pattern of stable and metastable configurations when r_{34} is equal to $2|\mathbf{b}_3|$, except there is a stable and attractive configuration at θ equal to 45˚. All of the other stable and metastable values of θ increase slightly except for 225˚. Table 1 also shows that when r_{34} is greater than or equal to $5|\mathbf{b}_1|$, the number of stable and metastable configurations is cut in half. Additionally, 45˚ is again a stable repulsive configuration at r_{34} equal to $5|\mathbf{b}_1|$ and $10|\mathbf{b}_1|$, while 225˚ becomes an attractive configuration at r_{34} equal to $10|\mathbf{b}_1|$. When r_{34} is greater than or equal to $20|\mathbf{b}_1|$, the stable and metastable regions are very similar to the scenario when there are just two dislocations moving towards a common junction without the influence of the sessile dislocation. The long range stress field of the sessile dislocation has very little influence on the glissile dislocations at these distances.

The nature of the repulsive and attractive junctions sheds new light on the requirements to form a cleavage crack in BCC materials based on the ability of glissile $\langle 111\rangle\{011\}$ dislocations to form a sessile dislocation at their common junction in the vicinity of a previously formed sessile dislocation. When r_{34} is $1|\mathbf{b}_1|$, there are no possible configurations where the glissile dislocations are mutually attracted to the common junction and an external stress is required to form sessile dislocations for a cleavage crack. As r_{34} increases past $20|\mathbf{b}_1|$, there are configurations where the dislocations are attracted towards the common junction without an external stress; however, the resulting sessile dislocations are not in as close proximity bringing the idea of forming a clearly defined cleavage crack as a direct result of these dislocation reactions somewhat into question. As a series of sessile dislocations begins to form, this analysis implies that sessile dislocations have very little influence on each other at distances greater than r_{34} equal to $20|\mathbf{b}_1|$, while sessile dislocations at distances less than $20|\mathbf{b}_1|$ can inhibit further sessile dislocation formation in the absence of an imposed external stress. One can envisage applying this analysis to observations of cleavage cracking in BCC materials. For example, Ogawa et al. [3] observed isolated cleave regions (ICRs) in pressure vessel steels; ICRs are regions of cleavage in between regions of fibrous fracture. The authors discussed the relationship between ICRs and particle clusters, but they may also be related to the cleavage cracking mechanism discussed in this paper. There is stress concentration around both particle clumps and fibrous fracture regions that could help overcome the repulsive stresses between glissile dislocations necessary to produce a cleavage crack in isolated and favorably oriented grains.

Summary

A. A method has been presented for rigorously computing interaction forces in BCC (and other) crystal structures.

B. Glissile $\frac{a}{2}\langle \mathbf{111} \rangle$-type dislocations are attracted to a common junction albeit in a complex manner.

C. The formation of cleavage crack nuclei requires stresses only as large as the lattice friction stress.

D. The interaction between sessile $a\langle 100 \rangle$ dislocations and glissile $\frac{a}{2}\langle \mathbf{111} \rangle$ pairs is such that there is almost never an attractive junction. Thus, additional work must be done to cause the growth of a cleavage crack.

E. The interaction between glissile and sessile dislocations is very sensitive to the distance between the existing and potential sessile dislocations.

References

[1] A.H. Cottrell: Trans. AIME Vol. 212 (1958), p. 192

[2] D. Li and M. Yao: Mat. Charact. Vol. 36 (1966) p. 27

[3] K. Ogawa, X.J Zhang, T. Kobayashi, R.W. Armstrong and G.R. Irwin: ASTM STP 833 (1984) p. 393.