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DISLOCATION EMISSION FROM CRACKS IN CRYSTALS OR ALONG CRYSTAL INTERFACES

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Introduction

A primary issue in the study of ductile vs. brittle crack extension concerns how adequate is the present understanding of the competition between cleavage decohesion and crack tip emission of blunting dislocations. The Kelly, Tyson and Cottrell approach (1), as refined in the Rice-Thomson model (2) and extensions to it (3-8), regards the outcome of this competition process as a fundamental measure of ductile and brittle material behavior. Specifically, materials are categorized as intrinsically cleavable if along a given loading path of an atomistically sharp crack, conditions for decohesion of the interface or crystal plane ahead of the crack are reached before those for dislocation emission from the crack. Conversely, a material is considered intrinsically ductile if dislocation nucleation conditions are reached first, whereby fracture is presumed to involve a ductile flow mechanism such as microvoid growth to coalescence and/or shear band localization. However, it is evident that evaluation of the competition process outlined provides an incomplete criterion to determine ductile and cleavage behavior. We enumerate some of the insufficiencies here by assuming that either dislocation emission or cleavage is the predicted outcome of the competition process described, and list the features and assumptions of the model which could alter the expected ductile or brittle crack tip response.

First, if dislocation emission is predicted to be favored by the Rice-Thomson model, the assumption that the crack tip is trapped by a potentially active slip plane should be questioned. Such a geometry seems to provide a most favorable condition for dislocation emission. In actuality, a macroscopic crack front may be arbitrarily oriented in the crystal, and ductile behavior may depend on whether the crack front is situated in a slip plane. However, crack nucleation mechanisms by dislocation pile-ups may favor such orientations.

Assuming again that emission is predicted to be favored, might a running crack introduced from a cracking brittle phase or perhaps an embrittled grain boundary move rapidly enough as to prevent sufficient crack tip blunting and relaxation of nearby stresses by a dislocation emission process? The motivation here arises from well known cases, notably for Fe alloys, where cleavage seems to result from crack injection from brittle carbides, and where the phenomenology of the ductile-brittle transition is explainable in such terms (e.g., Hahn (9)). Unfortunately, no definitive analysis of the emission versus cleavage competition is yet available for a rapidly moving crack. However, as commented upon and analyzed approximately by Jokl, Vitek and McMahon (10), the tradeoff of cleavage and dislocation emission may be related to the mobility of freshly nucleated dislocations, which must move away from the the crack tip and be followed by others in order to successfully relax near crack tip stresses. A nucleation problem yet to be fully addressed would focus on cases where there are limited external (non-crack-tip) dislocation sources to operate in the vicinity of a fast moving crack; here, crack tip emission, and thus the relaxation of stresses ahead of the crack, are limited by the rate at which dislocations may be continuously nucleated and moved away from the crack tip as it propagates or is further loaded.

On the other hand, if cleavage is favored in the competition process, are microstructural features such as brittle phase particles or regions affected by corrosive environments present to enable nucleation of an atomistically sharp crack, as postulated in the analysis? Dislocation motion near a potential nucleation site may prevent the build up of internal stresses needed for crack nucleation. Thus, although cleavage may be predicted, actual material behavior may depend on the probability that atomistically sharp cracks can be nucleated, which may then be related to slip character (e.g., planar versus wavy) and to factors such as alloying solutes and precipitates, prior work hardening, temperature, loading rate, etc., which control plastic strength and hence the generation of large internal stresses.

In a related manner, cleavage may be favored by the model, but for the actual crack, nearby dislocations may move from pre-existing sites and sources, as to intersect and blunt the crack tip, or to sufficiently reduce near tip stress such that a Griffith condition can not be met. In particular, observed cleavage to ductile transitions associated with temperature increases or loading rate decreases may generally be explained by

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assuming that the material involved is intrinsically cleavable at all temperatures. As the parameters entering the Rice-Thomson model have only modest temperature dependence, such a predicted favoring of cleavage is unlikely to be reversed with temperature. However, actual cleavage will be strongly temperature (and loading rate) dependent because these factors first determine if suitable internal stresses can first be formed to nucleate cracks, and second, control the generation and motion of externally (i.e., non-crack-tip) nucleated dislocations which can blunt or stress-relieve the crack. Studies by Hart (11) and Freund *et al* (12,13) have used a visco-plastic material behavior with the aim to understand effects of the mobility of non-tip nucleated dislocations on relaxing stresses near a moving crack tip. Given the high stresses near a crack tip loaded towards its Griffith limit, lattice defects which are relatively ineffective as sources under the normal stress levels of plastic flow could act as nucleation sites, at high temperature or low loading rate, and spoil the stress concentration.

Some noteworthy experiments indicate that the outcome of dislocation emission versus cleavage behavior may be more complex. As summarized recently by Argon (14), there is evidence that dislocations can be nucleated directly from crack tips, or from very-near-tip defects, in Fe, W, LiF and Si. However, these materials can cleave, and in the case of Si at elevated temperatures, this cleavage may have followed prior dislocation emission. It is unclear what role external, non-tip-nucleated dislocations have played here, but such observations suggest that dislocation emission, although favored initially, may not occur indefinitely. In addition, Vehoff, Neumann and Rothe (15-18) have interpreted their experiments on Fe-3% Si as showing that the amount of dislocation blunting and cleavage cracking can be varied continuously by temperature change and/or hydrogen partial pressure. This suggests that dislocation emission and cleavage cracking may alternate as the crack extends, or that perhaps they occur simultaneously and are not mutually exclusive processes, although again, it is unclear whether it is tip-nucleated dislocations or those from near-tip sources which are active. Nevertheless, the experiments of Ohr and coworkers, as summarized in (6), suggest that there is a critical load at a crack tip described in K_1, K_2, K_3 space at which dislocation emission is possible. We develop this concept as suggested by Rice and Thomson, and as developed by by Yokobori *et al* (4) in application to fatigue crack growth and by Rice (3) and Mason (5) for interfacial cracks, and as summarized recently by Lin and Thomson (8). Extensions are made here to include elastic anisotropy effects and to develop criterion for the unstable emission of a pair of partial Burgers vector dislocation loops from a f.c.c. crack tip. Emission is viewed in terms of a critical load set of local K values, and is discussed as a function of crystallographic orientation and the type of crack tip loading. The importance of crystal elastic anisotropy is discussed as well.

Development

The Rice-Thomson approach is described here by considering a plane crack, as in fig. 1, situated on a symmetric tilt crystal interface, or contained completely within a single crystal. The symmetric tilt configuration has no oscillating singularity (see (19,20)) that is usually present in the interfacial crack tip stresses. The crack front lies in a potentially active slip plane(s) inclined at angle ϕ to the uncracked extension of the crack plane. The local elastic stress field, which may be altered from the far field by dislocation shielding effects, is described in terms of a set of stress intensity factors K_1, K_2, K_3. The energy U associated with a half circular dislocation loop of radius r and Burgers vector b on the slip plane is (see fig. 1):

$$U = \pi r \left[\overline{E}_{core} + \alpha b^2 \ln(8r/e^2 b)\right] + 2r E_{ledge} - 3.5 b r^{3/2} K_i S_i \qquad (1)$$

Here $\overline{E}_{core}$ and E_{ledge} are respectively the core energy per unit length, averaged over the dislocation loop, and the ledge energy per unit length along the blunted crack front. The bracketted expression is an approximate representation of the dislocation self energy. It represents one-half the energy of a full circular dislocation loop on the same slip plane in an infinite, homogeneous, uncracked crystal. αb^2 is the prelogarithmic energy factor for a straight dislocation line with the same Burgers vector as the loop, averaged over all possible orientations of the line within the slip plane. α is calculated in the literature for slip systems in many cubic and h.c.p. materials (21), and for an isotropic solid, it is approximately (shear modulus)/10. The proceedure of using half the full loop energy exactly characterizes the force, dU/dr, resisting enlargement of a very long rectangular loop of short dimension r and with long axis parallel to the crack front; it is based on an exact 2-D calculation (22) of the force on a dislocation line parallel to the tip of a notch or crack, lying on an interface between arbitrarily oriented anisotropic single crystals. For the semicircular case discussed here, the proceedure represents an approximation which in principle can be improved by 3-D weight function techniques (23).

The geometrical factors S_i are defined such that $K_i S_i \rho^{-1/2}$ (summation over loading modes i=1,2,3) is the shear stress exerted on the slip plane in the slip direction, at distance ρ from the crack tip. The S_i can be computed from anisotropic elastic crack tip analysis for the intracrystalline (24) and intercrystalline (20) cases. The parameters S_i and E_{ledge} are sensitive to the orientation angles ϕ and ψ, of the slip system relative to the cracked interface, but α and $\overline{E}_{core}$ are not. In addition, S_i and α are well known from anisotropic elastic crack and dislocation theory, whereas E_{ledge} and $\overline{E}_{core}$ are poorly known.

The critical combination of K_i at which dislocation emission is spontaneous is calculated as follows (5): The equlibrium size of an incipient loop is given by $dU/dr = 0$, and this equilibrium condition becomes unstable as the sign of d^2U/dr^2 changes from (+) to (-). Using eqn.(1), we set $dU/dr = d^2U/dr^2 = 0$ to obtain the critical loading and loop radius as

$$\frac{K_i S_i}{\alpha b^{1/2}} = 0.76 \exp\left[(\pi \overline{E}_{core} + 2E_{ledge})/2\pi\alpha b^2\right] \quad ; \quad r = 2.51\, b\, \exp\left[-(\pi \overline{E}_{core} + 2E_{ledge})/\pi\alpha b^2\right] \tag{2}$$

This critical load set for nucleation is to be compared to that for cleavage decohesion of the interface, which is calculated by equating the elastic energy release rate G to 2γ, the work of interface separation against cohesive forces. Using the Willis solution for a 2-D interfacial crack bounded by elastic media (20),

$$G = (1/8\pi) K_i \alpha_{ij}^{-1} K_j = 2\gamma, \tag{3}$$

where α_{ij}^{-1} is extracted numerically using (20), and is the inverse of α_{ij} appearing in the prelogarithmic energy factor $b_i \alpha_{ij} b_j$ for a dislocation line with Burgers vector components b_i, that lies on the interface and is parallel to the crack front. The indices i,j =1,2,3 sum over the crack tip loading modes 2,1,3 respectively. For the special case of cracks on symmetric tilt boundaries and intracrystalline cracks in orientations of high symmetry, α_{ij} is a diagonal matrix. The α_{ij} generally vary modestly with crack orientation to the adjoining cubic crystals, although variation by as much as a factor of 2 is seen for some particular orientations.

For f.c.c. materials, it may be easier to nucleate partials from the crack tip rather than full Burgers vector dislocations. The formulation here is more elaborate, and requires, for nucleation of the first partial dislocation, adding an energy term $(\pi r^2/2)\gamma_{sf}$ to eqn.(1), where γ_{sf} is a stacking fault energy. Further, b as well as other parameters involved in eqn.(1) must be interpreted consistently for the first partial Burgers vector. For nucleation of the second partial, one must incorporate in addition a dislocation-dislocation interaction term as the second of the partials forms in the presence of the first. We base the dislocation energies and hence interactions on one-half the energy of a circular loop (first partial) containing within it a smaller concentric circular loop (second partial), using a solution by Lardner (25). The analogous approximation tests well for straight dislocation lines, parallel to the tip, where exact elasticity solutions can be derived (e.g., (8)).

Critical loads can be calculated for unstable emission of the first partial, as well as for the second partial in the presence of the first. Let r_* be the critical loop size as calculated from eqn.(2) when γ_{sf} is neglected, but with $b, \overline{E}_{core}, E_{ledge}$, etc., chosen as appropriate for the partial. Then we find the following: For $e\gamma_{sf}r_*/\alpha b^2 < 1$, the first partial suddenly pops out to an equilibrium loop size at a critical K after which, depending on material and geometric parameters, the second partial may either follow spontaneously or is nucleated upon further increase in K. For $e\gamma_{sf}r_*/\alpha b^2 > 1$, the first partial loop enlarges continuously, without unstable pop-out, with increasing K until at a critical level, the second partial nucleates. The nucleation of the second partial annuls the stacking fault and allows the resulting full dislocation loop to expand to large size. The critical load required to nucleate both partials is compared with that calculated for the full Burgers vector case. Our calculations for mode 1 loading of a crack on the (100) crystallographic plane, with crack front along [011], show partials to be more difficult to nucleate in Ag, Cu, Ni and Al. We find for Ag, Cu and Ni that $e\gamma_{sf}r_*/\alpha b^2 < 1$, and that the second partial is nucleated only upon further increase (typically 50%) in K. For Al, we estimate $e\gamma_{sf}r_*/\alpha b^2 > 1$, so that the stable enlargement of the first partial is predicted.

Discussion

Presented in fig. 2 are theoretical predictions for interfacial cracks loaded in mode 1 tension on several pure Cu- [110] symmetric tilt boundaries, with crack front notched along the [110] direction as to lie in an available {111} type slip plane. Here, G^{diel} (proportional to K^2 through eqn.(3)) is based on the full dislocation mechanism, and is presented against estimates of $G^{cleav} = 2\gamma$ for $T = 293K$. The line $G^{diel} = G^{cleav}$ in fig. 2 denotes the boundary between ductile and brittle behavior for an exact model. Our interest in presentation of results in fig. 2 is for other work, to be reported elsewhere, in which the effects of an embrittling grain boundary segregant (Bi in Cu) are to move the point for a given grain boundary relative to the ductile/brittle dividing line, principally by reducing 2γ.

Estimates of $G^{cleav} = 2\gamma$ are given by $2\gamma_s - \gamma_{gb}$, where γ_s , γ_{gb} are respectively the free energies per unit area of a pure Cu surface and grain boundary, evaluated at $T = 293K$. As surface energy measurements for Cu at 1200K are seen to vary with orientation by less than 5%, we use an estimate by Tyson (26) of $\gamma_s = 1.74 J/m^2$ for the average surface value at $T = 293K$. Accurate room temperature estimates are difficult due to a lack of knowledge of $d\gamma_s/dT$ as a function of T and the crystallographic surface. Grain boundary energy estimates are

made using values of relaxed energy for Cu [110]-symmetric tilt boundaries obtained by Wolf (27) by means of a pair spline potential for Cu. Although absolute energy values given here may not be accurate, we regard these results as a useful measure of relative grain boundary energy at 0K, and rescale them such that an average value of $\gamma_{gb} = 0.625 J/m^2$ reported by Murr (28) is obtained, using $d\gamma_{gb}/dT = -10^{-4} J/m^2 K$ as also given by Murr. The variation in 2γ with orientation in fig. 2 is then due solely to the variation in γ_{gb}.

Of the parameters used in eqn.(2) to calculate K_1^{disl}, $\overline{E}_{core}/\alpha b^2 = -0.205$, using an estimate from Prinz *et al* (29) consistent with a full Burgers vector cutoff, and $\alpha b^2 = 3.07 \cdot 10^{-10} J/m$ from (21) for a Cu (111) $\frac{1}{2}[1\bar{1}0]$ dislocation. E_{ledge} is approximated from (2) as $\gamma_{ledge} b \cos\psi \sin\phi$, where γ_{ledge}, the free energy per unit area of ledge, is estimated as $0.1\gamma_s$ using a Terrace-Ledge-Kink model to interpret experimental data for the change in γ_s with surface orientation (J.-S. Wang, private communication). The value of α_{22}^{-1} used in eqn.(3) has modest variation for the orientations presented, and is $\approx 1.7 \cdot (10^{10} Pa)^{-1}$.

We allow for a crack to be cut in either of two opposite crystallographic directions in the boundary, of type $[n\bar{n}\bar{m}]$ (denoted here by (+)) or $[\bar{n}nm]$ (denoted by (-)). An example of such directional dependence is seen for the Cu $(2\bar{2}1)[110]$ symmetric tilt boundary. Of the two opposite directions to notch the crack, the (-) direction (i.e, $[\bar{1}14]$) crack is predicted to respond in a ductile manner, whereas the (+) direction (i.e., $[1\bar{1}4]$) crack is predicted to cleave. Such an effect is due solely to the changes in E_{ledge} and S_1 caused by the different angles ϕ associated with the available {111} type slip planes. Specifically, the variation in G^{disl} is largely due to the change in the resolved shear stress factor S_1 through the dependence $K_1^{disl} \propto 1/S_1$ ($G^{disl} \propto 1/S_1^2$). Thus, G^{disl} is lowered when S_1 is maximized (at $\phi \approx 70°$, according to isotropic elasticity). Prior crack tip dislocation emission will shield the crack tip, as discussed by Sinclair and Finnis (30), and the shielding of the mode 1 stress intensity factor scales linearly with S_1 (2). Presumably, the mode 2 shielding factors will be small, assuming equal participation of the symmetrically oriented slip planes above and below the crack plane.

The effect of including elastic anisotropy in the competition process is seen to enter largely through the parameters S_i. An example of this may be seen in comparing S_1 for mode 1 loading of cracks in crystals with front aligned to $[1\bar{1}0]$, and the crack plane either (001) or (110) (the choice of two opposite crack extension directions is irrelevant here). The former crack plane orientation has been frequently cited with ductile extension in pure Cu single crystals, while the latter crack plane orientation has been observed in Cu and Cu alloys affected by stress corrosion cracking (31,32). Using isotropic elastic crack mechanics, the ratio of $(1/S_1)$ (to which K_1^{disl} is directly proportional) for the (110) crack plane to that for the (001) crack plane is 1.32 whereas the ratio calculated from anisotropic elasticity using proceedures of (24) is 1.08. In this case, use of isotropic elasticity would substantially overestimate the difference in K^{disl} values for the crack plane orientations discussed.

Ohr *et al* (6) in their electron microscope studies of crack tip deformation in several f.c.c. and b.c.c. materials frequently observed a combined mode 1 and mode 3 loading for cracks along crystal slip planes. The latter mode seemed most important in that screw dislocations with Burgers vector parallel to the crack front were often introduced onto a plane that is coplanar with the crack. S_3 is a maximum and $S_1 = 0$ for the slip plane in which the crack lies, so that the nucleation criterion as expressed in eqn.(2) is a function only of the mode 3 loading. Further, a comparison shows K_3^{disl} for this coplanar geometry to be much lower than K_1^{disl} for the mode 1 {001} crack plane geometries commonly observed in f.c.c. and b.c.c. materials. This is due largely to the higher value of S in the coplanar geometry, but also to the absence of a ledge term in this geometry, as the full Burgers vector is parallel to the crack front.

The present observations of Ohr *et al*, as reviewed in (6), suggest that there is a critical load at which crack tip dislocation emission occurs. Those authors have inferred values of K_3^{disl} for several f.c.c. and b.c.c. materials using a somewhat idealized model of their experiments, together with experimentally determined input parameters (size of dislocation free zone, presumably at incipient nucleation; size of pileup ahead of crack; yield stress for piled up group). Assuming such estimates to be correct, one may infer values of the poorly known core term. For the full Burgers vector loop, we may solve for the inferred core energy, $\overline{E}_{core}$, conveniently stated as a core cut-off radius r_0 ($\overline{E}_{core} = \alpha b^2 \ln(b/r_0)$), by eliminating the ledge term, which is not present in this full Burgers vector geometry, and inverting eqn.(2),

$$r_0/b = \exp\left(\frac{-\overline{E}_{core}}{\alpha b^2}\right) = \left(0.76 \frac{\alpha b^{1/2}}{K_3 S_3}\right)^2 \tag{4}$$

Table 1 shows the inferred values of r_0/b for full dislocations, using eqn.(4) with K_3^{disl} as estimated by Ohr *et al*. Uncertainties in the energy of the ledge structure produced by the first partial make inference of a partial core cut-off difficult. For f.c.c. materials, estimates of r_0/b are compared to those presented by Prinz *et al* (29), who use a nonlinear Peierls-Nabarro model which principally requires the value of $\gamma_{sf}/C_{44}b$ to determine r_0/b,

TABLE 1: A Comparison Of Core Cutoff Parameters

mat.	(exp. K_3)*	(αb^2)†	b	$\left(\frac{\alpha b^{1/2}}{K_3 S_3}\right)^{\ddagger}$	r_0/b values using eqn.(4)	r_0/b values from (29)
S.S	0.16	4.59	2.48	1.8	1.9	1.8
Al	0.07	2.15	2.85	1.6	1.5	0.49
Cu	0.04	3.07	2.55	4.7	13.00	1.2
Ni	0.14	5.03	2.49	2.3	3.1	0.89
Nb	0.14	3.35	2.86	1.2	0.83	
Mo	0.92	8.90	2.73	0.54	0.17	
W	1.4	11.4	2.74	0.44	0.11	

* from (6); in units of $MPa\sqrt{m}$

† from (21); in units of $10^{-10} J/m$

b in units of $(10^{-10} m)$

‡ $S_3 = 1/\sqrt{2\pi}$

where C_{44} is the elastic shear modulus. The results show rather large differences in the two estimates. The r_0/b values inferred from the Ohr *et al* data are consistently larger for the f.c.c. materials presented, and thus, are associated with consistently lower values of K_3^{disl} than would be calculated using the Prinz *et al* results. Further, there is considerable variation of the inferred r_0/b about the frequently assumed values of 2/3 for b.c.c. and 2 for f.c.c. materials, although these inferred values are lower for b.c.c. than for f.c.c. materials. The inferred r_0/b for Cu is implausibly large. This large variation in r_0/b (or equivalently $\overline{E}_{core}/\alpha b^2$) can make substantial changes in the predictions of $K_i S_i/\alpha b^{1/2}$, as presented in eqn.(2). For example, if the Prinz *et al* r_0/b values for Cu are used in eqn.(2) (neglecting ledge energy), then K_3^{disl} are respectively 0.13, 0.14 $MPa\sqrt{m}$ for the full and partial dislocation mechanism, as compared to 0.04 $MPa\sqrt{m}$ measured by Ohr *et al*.

Conclusions

We have presented an updated version of the Rice-Thomson calculations, taking fuller account of elastic anisotropy, stacking faults, etc. At best, the comparison of G^{disl} with G^{cleav} serves to show that a given lattice or grain interface is intrinsically cleavable. Actual behavior in cleavable solids may be dominated by surrounding crack tip deformation from external dislocation sources, and such considerations seem to explain the rate and temperature dependence of crack response in some materials. If one is to evaluate the cleavage versus emission competition, it is clear from considerations made here that material specific features such as the crystallographic orientation of the the crack plane and the direction of crack propagation, are important as are, in general, anisotropic elastic effects.

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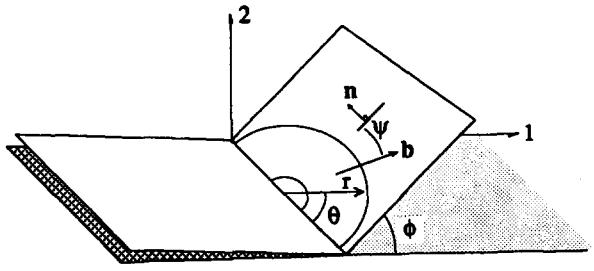

FIG. 1. Crack and Slip Plane Geometry.

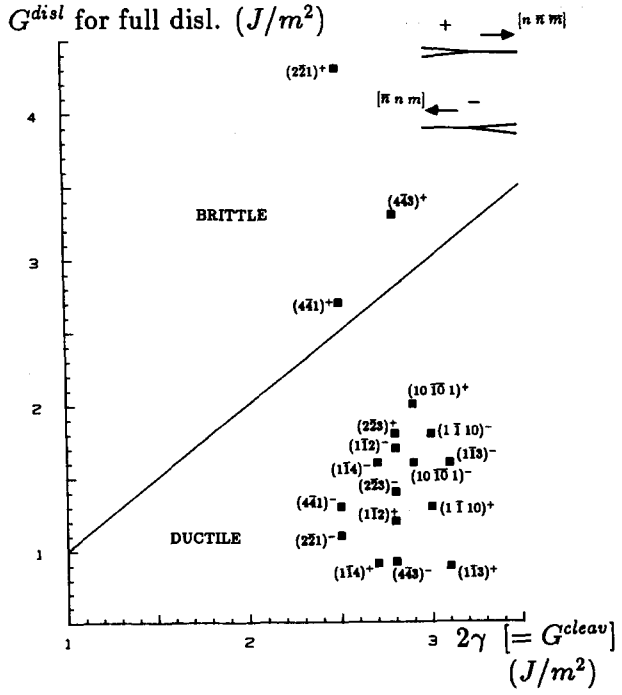

FIG. 2. Predictions for Pure Cu [110] Symmetric Tilt Boundaries at $T_{test} = 293K$.