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**ON THE ESCAIG OBSTACLE HYPOTHESIS FOR
CROSS-SLIP IN FACE-CENTERED-CUBIC MATERIALS
(POSTPRINT)**

**D.M. Dimiduk and C. Woodward
AFRL/RXCM**

**S.I. Rao and T.A. Parthasarathy
UES, Inc.**

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WRIGHT-PATTERSON AIR FORCE BASE OH 45433-7750
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Metals Branch
Structural Materials Division

//Signature//

DANIEL J. EVANS, Chief
Metals Branch
Structural Materials Division

//Signature//

ROBERT T. MARSHALL, Deputy Chief
Structural Materials Division
Materials And Manufacturing Directorate

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On the Escaig obstacle hypothesis for cross-slip in face-centered-cubic materials

S.I. Rao^{a*}, D.M. Dimiduk^b, C. Woodward^b and T.A. Parthasarathy^a

^aUES, Inc., 4401 Dayton Xenia Rd, Dayton, OH 45432 1894, USA; ^bAir Force Research Laboratory, Materials and Manufacturing Directorate, AFRL/MLLM Wright Patterson AFB, OH 45433 7817, USA

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There is a significant body of literature wherein a linear approximation of Escaig's model is used to justify the large experimentally measured activation volumes for cross slip in face centered cubic copper. Here, by examining the error between the linear approximation and the original theory, we show that this explanation is not satisfactory. The calculated value for activation volume in copper, using Escaig's original equations, yields $\sim 60b^3$ (b Burgers vector) while the linear approximation yields $200b^3$, the latter result fortuitously matching the experimental values.

Keywords: cross slip; activation volume; analytical equations; copper; glide stresses

1. Introduction

The early work of Escaig remains the most widely cited and used model for cross-slip [1–4]. To rationalize the much lower activation energies observed in experiments, this model was extended to include an ad-hoc postulate that obstacles always exist in materials which enable sufficient dislocation core constriction under stress, thereby reducing the activation energy for cross-slip [2]. This postulate or hypothesis was also invoked by Bonneville and Escaig [2] to explain the high activation volumes observed for cross-slip in specialized cross-slip deformation experiments. Unfortunately, this rationalization included a linear approximation of the original Escaig model. In this note, we explore this hypothesis by using the original Escaig model (without the linear approximation). We find that there are significant errors in linear approximation, and further that the complete model leads to a significantly lower theoretical cross-slip activation volume compared to the experimental one. We thereby suggest that the high activation volumes observed for cross-slip in cross-slip deformation experiments of copper remain unexplained.

*Corresponding author. Email: satish.rao@wpafb.af.mil

2. Analysis

Bonneville and Escaig [2] measured an activation volume for cross-slip in FCC Cu to be fairly high, $\sim 300b^3$, using specialized cross-slip deformation experiments. The activation volume for cross-slip with respect to Escaig stresses – the stresses that significantly modify the activation energy for cross-slip in FCC materials [3,4] by changing the dislocation core width – is known to be an order of magnitude lower [1–5]. Further, the activation volume for cross-slip with respect to Escaig stresses is negative in tension, that is, increasing Escaig stress increases the activation energy for cross-slip in tension. As a result, Bonneville and Escaig [2] postulated the obstacle hypothesis: cross-slip in FCC materials always occurs at some unknown obstacles where the screw dislocation is completely blocked. Since the screw dislocation is completely blocked, the applied glide stresses alter the force equilibrium at the screw dislocation, resulting in a smaller activation energy for cross-slip. This decrease in activation energy has been estimated by Bonneville and Escaig, approximate to linear terms in the applied stress. The altered force equilibrium at the screw dislocation in the presence of the applied stress with the screw dislocation completely blocked at an obstacle can be written as

$$F_{\text{int}} = \gamma + \tau b/2, \quad (1)$$

where τ is the resolved shear stress on the glide plane, γ the stacking fault energy, and F_{int} the interaction force between the Shockley partials at equilibrium. Therefore, the effective stacking fault energy at the screw dislocation becomes

$$\gamma_{\text{eff}} = \gamma + \tau b/2. \quad (2)$$

This produces a smaller Shockley partial splitting at the screw dislocation. The ratio of the Shockley partial splitting distance on the cross-slip plane (d , where the screw dislocation is not blocked) to the Shockley partial splitting on the glide plane (d') is simply

$$d/d' = (\gamma + \tau b/2)/\gamma = 1 + \tau b/2\gamma. \quad (3)$$

Writing d' as $d - \Delta d$, where Δd is the change in the Shockley partial splitting due to the applied stress, one can rewrite Equation (3) as

$$\Delta d/d \sim \tau b/2\gamma. \quad (4)$$

The critical resolved shear stress for cross-slip as measured by Bonneville and Escaig [1,2] ranges from 25–40 MPa and the stacking fault energy of Cu is $\sim 44 \text{ mJ/m}^2$ [6]. For such cross-slip stresses, the effective stacking fault energy changes from 44 mJ/m^2 to $\sim 47\text{--}49 \text{ mJ/m}^2$, which is approximately an 8–11% change. One notes that such small changes in effective stacking fault energy can probably occur due to other reasons along the screw dislocation line, for example, the presence of vacancy or interstitial or foreign atom clusters; however such changes need to occur preferentially on the glide plane. Bonneville and Escaig expressed the activation energy for cross-slip, with the screw dislocation blocked at an obstacle (approximate to linear terms in the applied stress and neglecting

Escaig stresses) as

$$\begin{aligned} W &\sim [A\mu b^2/8\pi]d[(1-b/d)^2 - 2.771\tau b/\gamma] \\ &\sim [A\mu b^2/8\pi]d(1-b/d)^2[1 - [2.771/(1-b/d)^2]\tau b/\gamma], \end{aligned} \quad (5)$$

where A is ~ 0.93 for a d/b ratio of 6 [1,2], $d/b \sim 6$ for Cu [7] and within elasticity theory, $\mu b^2/16\pi\gamma = d$. Substituting Equation (4) into Equation (5), Equation (5) can be rewritten as

$$W \sim 2Ad^2(1-b/d)^2\gamma[1 - [5.543/(1-b/d)^2]\Delta d/d]. \quad (6)$$

From Equation (6), for an 8–11% change (3–5 mJ/m² change) in the effective stacking fault energy ($\Delta d/d \sim 0.08$ – 0.11) the cross-slip activation energy decreases from 0.83 eV to 0.30–0.10 eV, a 64–88% decrease ($d/b = 6$). These results seem unphysical; such small changes in effective stacking fault energy are not expected to lead to such substantial changes in the cross-slip activation energy. However, the cross-slip activation energy at zero stress, 0.83 eV, is in reasonable accord with recent atomistic simulation results, ~ 0.85 eV [6]. The use of continuum theory for this problem is problematic; however, since the continuum theory appears to predict the correct activation energy at zero stress and an exact atomistic calculation of the cross-slip activation energy under stress appears infeasible, we will apply the exact Escaig continuum equations to determine the effect of applied stress on cross-slip activation energy.

From Equations (5) and (6), the activation volume for cross-slip, $V = -dW/d\tau$, is simply

$$V = -\partial W/\partial\tau \sim 5.543Ad^2b. \quad (7)$$

The activation volume at a d/b ratio of 6 is $\sim 200b^3$ which is fairly close to the experimentally measured activation volume of $300b^3$. However, as noted previously, the activation energy decrease due to applied stress seems unphysical and one needs to consider cross-slip activation energy equations without the linear approximation. According to Caillard and Martin [4], the Escaig equations [3] for cross-slip activation energy can be written as

$$W = U_{\text{constr}} + L\Delta E, \quad (8)$$

where

$$U_{\text{constr}} = (A\hat{T})^{1/2}(1 + E/\hat{T}) \int_b^{d_M} [f(x) - f(d_M)]^{1/2} dx \quad (9)$$

and

$$L = (\hat{T}/A)^{1/2} \int_b^{d_M} [f(x) - f(d_M)]^{1/2} dx \quad (10)$$

and

$$\Delta E = Af(d_M), \quad (11)$$

Table 1. δ as a function of d/d' , evaluated by Escaig [3] and Caillard and Martin [4].

d/d'	1	1.001	1.01	1.03	1.083	1.11	1.28	1.71	2.53	3.57	6.73
δ	0.008	0.028	0.087	0.167	0.279	0.311	0.479	0.663	0.794	0.861	0.93

where

$$\begin{aligned} f(x) &= -\ln(x/d) + x/d - 1 + \ln(d'/d) \\ \ln(d/d') &= -\ln(d_M/d) + d_M/d - 1 + 0.155\delta. \end{aligned} \tag{12}$$

The function δ has been defined by Escaig [3] as

$$\delta = \int_0^{d_M} [f(x) - f(d_M)]^{1/2} dx / \int_0^{d_M} (1-x)^2 [f(x) - f(d_M)]^{1/2} dx \tag{13}$$

and

$$\begin{aligned} d(A\hat{T})^{1/2} &= (\mu b^3/8\sqrt{3\pi})(d/b)[\ln(d\sqrt{3}/b)]^{1/2} \\ &\sim (2/\sqrt{3})d^2\gamma[\ln(d\sqrt{3}/b)]^{1/2}. \end{aligned} \tag{14}$$

The values of δ for various values of d/d' has been tabulated by Escaig and Caillard and Martin and is shown in Table 1. E and T are the energy per unit length and the effective line tension of the Shockley partials, respectively and $E \sim 0.7T$. Equations (8)–(14) show that for a d/d' of 1 (zero stress), the activation energy for cross-slip in Cu is 0.62 eV ($d/b=6$, $\gamma=44$ mJ/m²), which is fairly close to the atomistic simulation result of 0.85 eV [6], whereas for a d/d' of 1.11 (11% change in the effective stacking fault energy), the cross-slip activation energy becomes 0.41 eV, only a 33% decrease in the cross-slip activation energy. From Equation (3), for a 11% change in stacking fault energy, the effective resolved shear stress is $\tau \sim 38$ MPa. Writing W as W_0 (value at zero stress) – $V\tau$, the effective activation volume, V for a 11% change in stacking fault energy becomes $\sim 52b^3$. Similarly, for a d/d' of 1.083, cross-slip activation energy is ~ 0.45 eV, $\tau=28.8$ MPa and effective activation volume, V is $\sim 57b^3$. However, for only a 0.1% change in effective stacking fault energy ($d/d'=1.001$), the effective activation volume becomes $\sim 200b^3$, in agreement with Bonneville and Escaig equations. This is illustrated in Figure 1, where the cross-slip activation energy, scaled to a value of 1 at a d/d' ratio of 1 (zero stress), is plotted against the d/d' ratio using the exact Escaig equations as well as the linear approximation for a d/b ratio of 6. Figure 1 clearly shows that the linear approximation breaks down significantly for the level of d/d' ratio reached in experiment ~ 1.11 . Note that in Figure 1, the fully constricted state for the screw dislocation was taken to be when the Shockley partial separation distance becomes ‘ b ’, the Burger’s vector of the screw dislocation whereas in [3, Figure 3], the fully constricted state was taken to be when the Shockley partial separation distance becomes zero. As a result, the cross-slip activation energy shows a steeper fall off with d/d' in Figure 1 as compared to [3, Figure 3].

These results show that when the exact equations derived by Escaig are used for the cross-slip activation energy, without the linear approximation, the activation

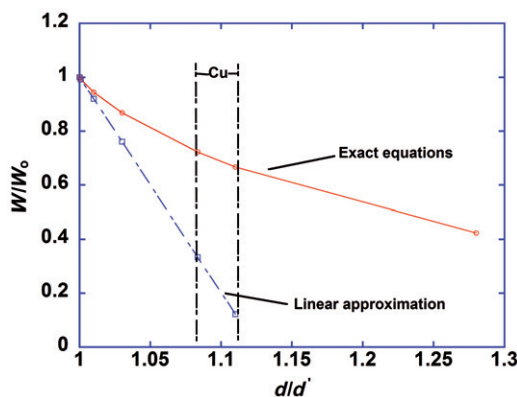


Figure 1. A plot of the activation energy for cross slip as a function of d/d' ratio for Cu, using the exact Escaig equations as well as the linear approximation of Bonneville and Escaig, for a d/b ratio of 6.

volume for cross-slip with respect to applied glide stresses with the obstacle hypothesis is only $\sim 60b^3$ for the level of cross-slip stresses reached in experiment. This is approximately a factor of 5 lower than experiment. Equations (8)–(14) also suggest that to explain the activation volume for cross-slip observed in experiments within the obstacle hypothesis, a d/b ratio of ~ 13 is required. However, in this case, the cross-slip activation energy at zero stress is predicted to be much too large for Cu, ~ 2.7 eV, as compared to atomistic simulation results [6] or experiment [2]. It is suggested that a different explanation is required for the high activation volumes for cross-slip observed in experiments. Recently, the authors proposed a mechanism for cross-slip predominantly occurring at screw dislocation intersections with forest dislocation obstacles [7] or, cross-slip preferentially occurring at screw dislocation dipoles blocked by some unknown obstacles [8]. These mechanisms may provide an alternate explanation.

3. Conclusions

For the levels of stress reached in cross-slip deformation experiments, the exact expressions derived for cross-slip activation energy by Escaig [3] and Caillard and Martin [4] need to be used. If the exact expressions are used, the cross-slip activation volume within the obstacle hypothesis is only $\sim 60b^3$ in Cu, a factor of 5 lower than experimental measurements. It is suggested that a different explanation is required for the high cross-slip activation volumes observed in experiments for Cu. Note that a recent experimental study [9] gives a corrected activation volume of $\sim 120b^3$ for cross-slip in Cu.

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