CONOIDAL CRACK WITH ELLIPTIC BASES, WITHIN CUBIC CRYSTALS, UNDER ARBITRARILY APPLIED LOADINGS - IV. APPLICATION TO ½<110> {111} CROSS-SLIP IN FCC MATERIALS

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ABSTRACT

Assuming the dislocation elliptical in the cross-slip plane at the beginning of the cross-slip process, it is shown that <*G*>, a measure of the energy release rate, obtained in *Part I* of this study applies. ½ <110> {111} cross-slip systems, observed in [112] copper single crystals deformed through *stage III* in constant strain rates above room temperature, do correspond to positive local <*G*> maxima. It is also suggested that the same treatment applies to the cross-slip between parallel basal planes in close packed hexagonal (CPH) structures.

Keywords : *fracture mechanics, linear elasticity, dislocations, crack extension force, high temperature mechanical twinning, cross-slip.*

RÉSUMÉ

Fissure conoïdale à base elliptique dans un cristal cubique sous sollicitations extérieures arbitraires – IV. Application au glissement dévié ½<110> {111} dans les matériaux CFC

En supposant la forme de la dislocation elliptique dans le plan de glissement dévié, au début du processus de déviation, il est montré que <*G*>, une mesure du taux de libération d'énergie obtenue dans la *partie I* de cette étude s'applique. Les systèmes de glissement dévié ½ <110> {111}, observés dans des monocristaux de cuivre d'axe [112] déformés au *stade III* à des vitesses de déformation constantes au-dessus de la température ambiante, correspondent à des maximas positifs locaux de <*G*>. Il est également suggéré que le même traitement s'applique au glissement dévié entre des plans basaux parallèles dans des structures hexagonales compactes (HC).

Mots-clés : *mécanique de la rupture, élasticité linéaire, dislocation, force d'extension de fissure, maclage mécanique à haute température, glissement dévié.*

I - INTRODUCTION

In the same way as in *Part II* and *III* [2, 3], the analysis of *Part I* [1] is applied to ½ <110> {111} cross-slip systems, observed in [112] copper single crystals deformed through *stage III* in constant strain rates above room temperature (present *Part IV*). We refer to the experimental works [4 - 7] and the stereographic projection with centre [112] ***(Figure 1)*** for the identification of slip systems. Plastic deformation of the specimens begins in *stage II* with the two symmetrical equally stressed slip systems ½ [011] $(1\bar{1}1)$ and ½ [101] $(\bar{1}11)$.

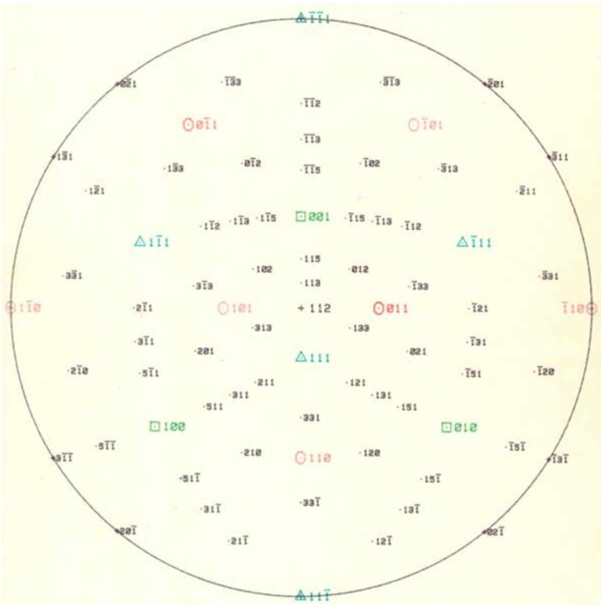

Figure 1 : *Stereographic projection with centre* [112] *for the identification of slip systems*

The hardening rate ($\theta = d\tau / d\gamma$; τ and γ, shear stress and strain) in *stage II*, θ_{II}, is constant with stress τ. At a stress level called τ_{III} begins the deformation stage *III* where θ_{III} is decreasing with stress [4 – 6]. Abundant cross-slips occur on the deviation plane $(11\bar{1})$ and these are due to screws ½ [011] and ½ [101] gliding initially on $(1\bar{1}1)$ and $(\bar{1}11)$, respectively [4, 7]. In this *part IV* and *Section* 2, the methodology for the use of the analysis in [1] is described. In *Section* 3, results are displayed corresponding to cross-slips. *Section* 4 and 5 concern discussion and conclusion, respectively.

II - METHODOLOGY

Figure 2 shows the conoidal crack geometry under load that has been used in [1] to calculate the associated crack extension force G per unit length of the crack front.

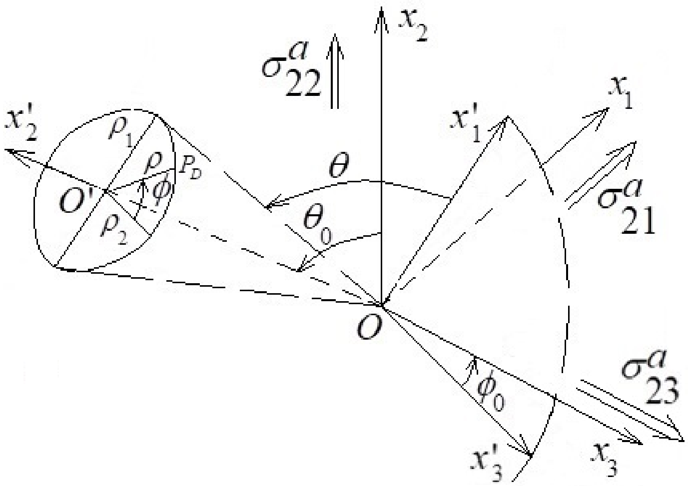

Figure 2 : *Elliptical base (elevation* $x_2^{'}$ *= OO'≡ h) of the conoidal crack with semiaxes* ρ_1 *and* ρ_2 *along* $x_1^{'}$ *and* $x_3^{'}$*.The running point* P_D [1] *along the base and angular parameters* θ_0 *and* ϕ_0 *that connect* $\mathbf{x}_j$ *and* $\vec{x}_j^{'}$ *are illustrated. Angle* θ *is introduced by the relation* $\tan\theta = OO'/\rho_1$. *The medium suffers uniformly applied tension* σ^a_{22} *in the vertical* x_2 *- direction and shears* σ^a_{21} *and* σ^a_{23} *(parallel to the horizontal* x_1x_3*- plane) in the* x_1 *and* x_3 *directions.*

Induced normal Poisson's stresses $-\nu_A(j)\sigma^a_{22}$ along x_1 (j=1) and x_3 (j=3) are included. The crack nuclei are arbitrarily oriented with attached Cartesian (*O;* $x_j^{'}$); $O\,x_2^{'}$ is a symmetrical axis. In $x_1^{'}x_3^{'}-$planes, the bases are elliptical with semiaxes ρ_1 and ρ_2 along $x_1^{'}$ and $x_3^{'}$ such that $a_r = \rho_1 / \rho_2$ = constant about any elevation $x_2^{'} = OO' \equiv h$ along $O\,x_2^{'}$. The angle ϕ is between $O'\,x_3^{'}$ and $O'P_D$ as shown in ***Figure 2***. Angle θ is measured in $O\,x_1^{'}\,x_2^{'}$ between $\boldsymbol{P_D}$ ($\phi = \pi/2$) ***O'*** and $\boldsymbol{P_D}$ ($\phi = \pi/2$) ***O*** where P_D ($\phi = \pi/2$) has elevation $x_2^{'} = h$ from $O\,x_1^{'}\,x_3^{'}$; its alternate interior angle is shown in ***Figure 2***. Additional angular parameters θ_0 and ϕ_0 (Euler's angles) are introduced that connect $\vec{x}_j$ to $\vec{x}_j^{'}$. We consider average <G>.

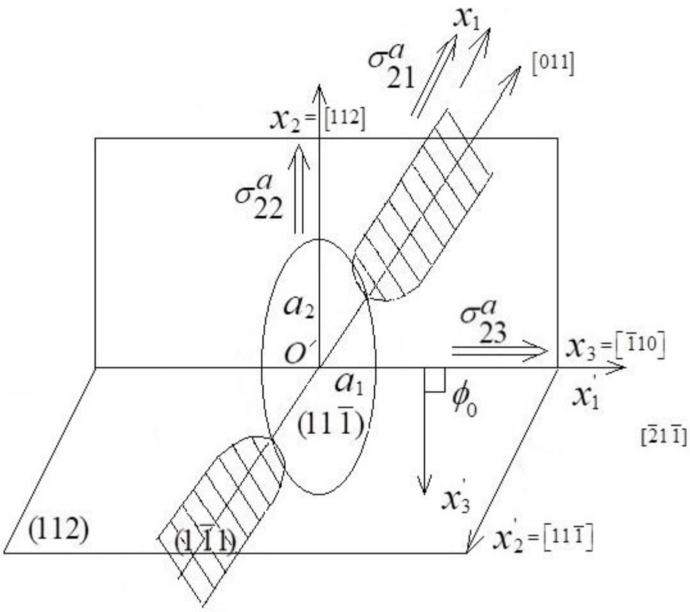

Figure 3 : *Configuration (at an arbitrary time t) of the screw dislocation* $1/2[011]$ *during the cross-slip process. The shape is assumed elliptical in* $(11\bar{1})$ *and the parts in* $(1\bar{1}1)$ *are hatched*

obtained in the first part of this study (see relation (34) of [1]) and present below graphical plots of its normalized value $<\tilde{G}_r>$ defined as

$$<\tilde{G}_r> = <G> / G^I_{Cs} = <\tilde{G}_r> (\theta, \theta_0, \phi_0, M_{12}, M_{13}, a_r, C_{nm}),$$
$$G^I_{Cs} = \frac{2^4 \alpha_0^2}{3\pi^2 C_{44}} (K^0_I)^2; \qquad (1)$$

where $K^0_I = \sigma^a_{22}\sqrt{\pi\Delta}$, $M_{12} = \sigma^a_{21} / \sigma^a_{22}$ and $M_{13} = \sigma^a_{23} / \sigma^a_{22}$; Δ is the separation of the partial dislocations. The applied stresses are viewed as effective stresses acting on the dislocations in the medium. The room temperature average values C_{11}= 1.691, C_{12}= 1.222 and C_{44} = 0.7542 in units of $[10^{11} N / m^2]$ for copper have been used (see *Table* 2 in [8]). ***Figure* 2** is used to specify a plane of cross-slip (S). x_2 is vertical, parallel to the applied tension, x_3 is then determined as the intersection between (S) and the laboratory horizontal plane (x_2) = Ox_1x_3 allowing x_1 to be known. For definiteness, x_2 is fixed to [112] and we seek possible cross-slip systems under such conditions. Then graphical plots of $<\tilde{G}_r>$ as a function of ϕ_0 are displayed. The cross-slip propagation directions [U] in (S) are those associated to positive local maxima. We take (S) = $(11\bar{1})$

[4, 7] : using ***Figure 1*** and ***2*** and indicating the directions only, we have

$$\theta_0 = \pi / 2 \, , x_2 = [112], \; x_3 = [\bar{1}10] \, , \; x_1 = [\bar{1}\,\bar{1}1] \, , \; x_2^{'} = [11\bar{1}] \qquad (2)$$

Figure 3 displays the configuration (at an arbitrary time *t*) of the screw dislocation ½ [011] during the cross-slip process. The shape is assumed elliptical in $(11\bar{1})$ and the parts in $(1\bar{1}1)$ are hatched. As the ellipse expands in $(11\bar{1})$, the configurations in $(1\bar{1}1)$ remain unchanged; consequently, these latter contribute non-additional value to $<G>$ ($d<G> = 0$) there. Hence, $<G>$ value is carried by the elliptical shape in $(11\bar{1})$. The quantity $<G>$ (see expression (34) in [1]) applies. Positive local maxima of $<\tilde{G}_r>$ correspond to equilibrium states of the cross-slip. The loadings are along x_j as indicated ***(Figure 3)***. $a_r = a_1 / a_2$, where a_1 and a_2 are the semiaxes along $x_1^{'} = [\bar{1}10]$ and $x_3^{'} = [\bar{1}\,\bar{1}\bar{2}]$, respectively. In the stationary configuration, we take $2a_2 = \Delta$ the separation of partials (1). The resolved shear stress τ_{III} at the beginning of *stage III* has been found thermally activated, satisfying an Arrhenius law temperature *T* dependence [4-6]. This can be included in the analysis in a similar way as for τ_V [2] the stress at the beginning of twinning.

III - RESULTS

Figure 4 is a plot of $<\tilde{G}_r>$ (1) for *(S)*= $(11\bar{1})$ (2) as a function of ϕ_0. Positive maxima of $<\tilde{G}_r>$ are at $\phi_0 = \pi / 2$ and π approximately (visual inspection). The former corresponds to the cross-slip system $[011](11\bar{1})$ ($\phi_0 = \pi / 2$). The second may be other mechanisms ($[\bar{1}\,\bar{1}\bar{2}](11\bar{1})$ twinning and fracture, for instance); these are observed at higher stress levels as compared to τ_{III} under similar temperatures. ***Figure 5*** shows $<\tilde{G}_r>$ (1) for the cross-slip system $[011](11\bar{1})$ ($\theta_0 = \pi / 2 \, , \phi_0 = \pi / 2$) as a function of a_r. Visual inspection shows non-negative values of $<\tilde{G}_r>$ close to zero, from $a_r \cong 0$ up to $a_r \cong 1.5$. Above 1.5, $<\tilde{G}_r>$ is clearly negative. A maximum positive $<\tilde{G}_r>$ value is expected about $a_r = 1$ which would be the value of a_r at the equilibrium state. $a_1 \cong a_2 \cong \Delta / 2$ is expected in the equilibrium configuration of the cross-slip mechanism ***(Figure 3)***. A further expansion of the loop from that position would correspond to $d < \tilde{G}_r >= 0$. Under such conditions, the cross-slip process is completed allowing motion of the perfect dislocation in the cross-slip plane. We stress that at the beginning of the cross-slip process ***(Figure 3)***, θ is expected to be close to $\pi / 2$; this is appreciated using ***Figure 2***.

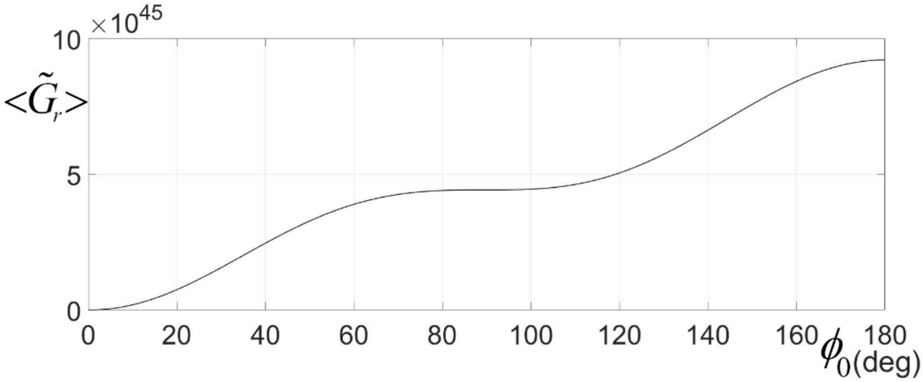

Figure 4 : $< \tilde{G}_r >$ (1) *as a function of* ϕ_0 *for* $\theta = \pi / 2$ *and* $\theta_0 = \pi / 2$. *This corresponds to the cross-slip system* $[011](11\bar{1})$ ($\phi_0 = \pi / 2$). $M_{12} = M_{13} = 10^{-4}$, $\nu_A(1) = \nu_A(3) = 1/3$, $a_r = 3 / 4$, *copper*

IV - DISCUSSION

Assuming the dislocation elliptical in the cross-slip plane at the beginning ***(Figure 3)***, $<G>$ obtained in [1] applies. Fixing $\theta = \pi / 2$ means maintaining a_1 close to zero ($a_1 \approx 0$) from the definition of θ [1]: we have $\tan\theta = OO' / a_1$ ***(Figure 2)***. At $\phi_0 = \pi / 2$ ***(Figure 3)***, the tensile stress along $x_3^{'}$ is $\sigma_{33}^{'A} = \sigma_{22}^{a}$ allowing a_2 to increase. Under such conditions, a_2 can be larger than a_1, meaning that $a_r = a_1 / a_2 < 1$. $< \tilde{G}_r >$ values in ***Figure 4*** conform to these conditions; positive local maximum of $< \tilde{G}_r >$ is at $\phi_0 = \pi / 2$. This is the equilibrium state $d < \tilde{G}_r >= 0$ of the cross-slip event. Another observed maximum is at $\phi_0 = \pi$. This would correspond to other mechanisms such as twinning and fracture. We can comment about the positive minimum of $< \tilde{G}_r >$

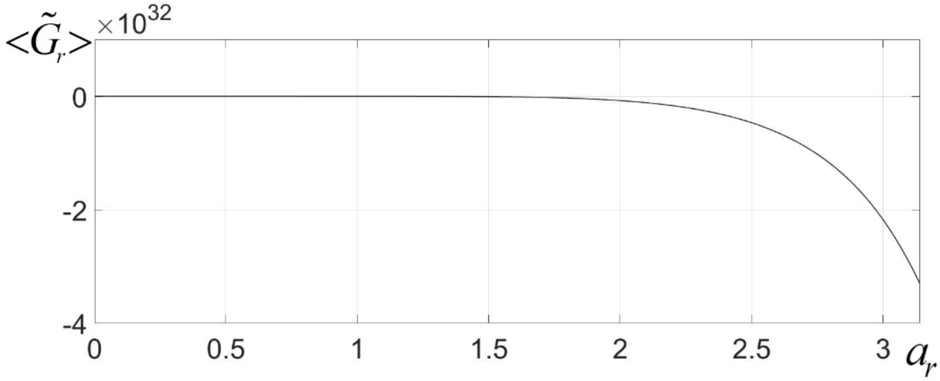

***Figure* 5 :** $<\tilde{G}_r>$(1) *as a function of* a_r *for* $\theta = \pi / 2$ *and the cross-slip system* $[011](11\bar{1})$ ($\theta_0 = \phi_0 = \pi/2$). $M_{12} = M_{13} = 10^{-4}$, $\nu_A(1) = \nu_A(3) = 1/3$, $a_r = 3/4$, *copper*

observed at $\phi_0 = 0$ ***(Figure 4)*** : using ***Figure 3***, the tension along $x_1^{'}$ is $\sigma_{11}^{'A} = \sigma_{22}^{a}$ allowing a_1 to increase, but this is hindered by the condition $\theta = \pi / 2$ $(a_1 \square 0)$; Poisson stress is compressive and reads $\sigma_{33}^{'A} = -\nu_A(3)\sigma_{22}^{a}$ hindering also the increase of a_2. Under such conditions $\phi_0 = 0$ is not favoured in ***Figure 4***. In summary, the analysis of *Part I* [1] predicts the observed cross-slip system $[011](11\bar{1})$ of the face-centred-cubic (FCC) structure using the configuration of the screw dislocation, at an arbitrary time *t*, given by ***Figure 3***. Earliest works [9 - 12] on cross-slip have used configuration like ***Figure 3***.

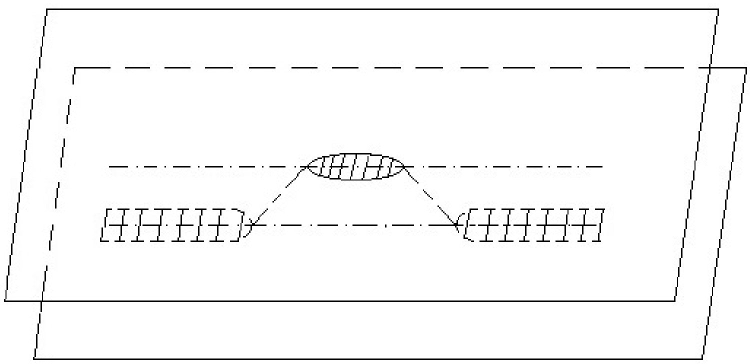

Figure 6 : *Configuration, under load, of the screw dislocation in the cross-slip process between basal planes of CPH structure*

We next make a discussion on cross-slip in close packed hexagonal (CPH) structure. A configuration under load, at a given time *t*, of the cross-slip event between basal planes is depicted in ***Figure 6***. The dissociation of the dislocation occurs in parallel planes. It is again assumed an elliptical shape for the dislocation on the cross-slip plane at the beginning of the process. The configuration out of the deviation plane remains unchanged during an increase of time *dt*; this means that $d < G >= 0$ there; hence the change in $<G>$ is entirely carried by the elliptical dislocation. This means that the treatment of *Part I* [1] applies for CPH structures. ***Figure 6*** is considered in previous works [13, 14].

V - CONCLUSION

Assuming the shape of the dislocation elliptical ***(Figure 3)*** in the cross-slip plane at the beginning of the cross-slip process, it is shown that $<G>$, a measure of the energy release rate, obtained in *Part I* [1] of this study applies. ½ <110> {111} cross-slip systems, observed in [112] copper single crystals deformed through *stage III* in constant strain rates above room temperature, do correspond to positive local $<G>$ maxima. It is also suggested that the same treatment applies to the cross-slip between parallel basal planes in close packed hexagonal (CPH) structures.

REFERENCES

[1] - P. N. B. ANONGBA, Conoidal crack with elliptic bases, within cubic crystals, under arbitrarily applied loadings – I. Dislocations, crack-tip stress and crack extension force, (a*) Rev. Ivoir. Sci. Technol.*, 43 (2024) 100 - 121; (b) *ResearchGate*, DOI: 10.13140/RG.2.2.21165.67044

[2] - P. N. B. ANONGBA, Conoidal crack with elliptic bases, within cubic crystals, under arbitrarily applied loadings – II. Application to mechanical twinning of [112] copper single crystals, (a*) Rev. Ivoir. Sci. Technol.*, 43 (2024) 122 - 131; (b) *ResearchGate*, DOI: 10.13140/RG.2.2.33154.70085

[3] - P. N. B. ANONGBA, Conoidal crack with elliptic bases, within cubic crystals, under arbitrarily applied loadings – III. Application to brittle fracture systems of $CoSi_2$ single crystals, (a*) Rev. Ivoir. Sci. Technol.*, submitted; (b) *ResearchGate*, DOI: 10.13140/RG.2.2.34719.37282

[4] - P. N. B. ANONGBA, Doctorate thesis No. 826, EPFL, Lausanne, (1989)

[5] - P. N. B. ANONGBA, J. BONNEVILLE and J.-L. MARTIN, Hardening stages of [112] oriented copper single crystals at intermediate and high temperatures, Proceedings of the 8th International Conference of the Strength of Metals and Alloys (ICSMA – 8), Tampere, Finland, Vol. 1, (1988) 265 - 270

[6] - P. N. B. ANONGBA, J. BONNEVILLE and J.-L. MARTIN, Hardening stages of [112] copper single crystals at intermediate and high temperature-I. Mechanical behaviour, *Acta metal. Mater.*, 41 (1993) 2897 - 2906

[7] - P. N. B. ANONGBA, J. BONNEVILLE and J.-L. MARTIN, Hardening stages of [112] copper single crystals at intermediate and high temperature-II. Slip systems and microstructures, *Acta metal. Mater.*, 41 (1993) 2907 - 2922

[8] - H. M. LEDBETTER and E.R. NAIMON, Elastic properties of metals and alloys. II. Copper, *J. Phys. Chem. Ref. Data*, Vol. 3, N°4, (1974) 897 - 935

[9] - J. FRIEDEL, “Dislocations”, Pergamon Press, Paris, (1964)

[10] - G. SCHOECK and A. SEEGER, Report of the Bristol Conference on Defects in Crystalline Solids, *Physical Society*, London, (1955) 340 p.

[11] - H. WOLF, *Z. Naturf. (A)*, 15 (1960) 180

[12] - J. BONNEVILLE, B. ESCAIG and J. L. MARTIN, A study of cross-slip activation parameters in pure copper, *Acta metall.*, 36 (1988) 1989 - 2002

[13] - M. S. DUESBERY and P. B. HIRSCH, in Dislocation Dynamics (Battelle Colloquium, Seattle-Harrison, 1967) Rosenfield, A. et al., Eds. (Mc Graw-Hill Book Co., New York), (1968) 57 p.

[14] - B. ESCAIG, L’activation thermique des déviations sous faibles contraintes dans les structures h.c. et c.c., *phys. Stat. Sol.* 28 (1968) 463 - 474