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CONOIDAL CRACK WITH ELLIPTIC BASES, WITHIN CUBIC CRYSTALS, UNDER ARBITRARILY APPLIED LOADINGS - III. APPLICATION TO BRITTLE FRACTURE SYSTEMS OF $CoSi_2$ SINGLE CRYSTALS

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ABSTRACT

Brittle fracture systems (<112> {111}, <113> {110}, <411> {122}) observed in $CoSi_2$ single crystals have been confronted to the theoretical analysis of *Part I* of this study. These do correspond to positive local average $< G >$ maxima, where the quantity $< G >$ is the crack extension force G per unit length of the crack front, averaged other all the positions on the crack front. Hence, equilibrium crack systems provided by the theory are those observed experimentally. Both twinning and cracking systems are of the type <112> {111} as expected. It is understood that above results are achieved within the framework of the theory of linear elasticity incorporating dislocations as crystal defects and basic elements in the mathematical treatment of fracture.

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

RÉSUMÉ

Fissure conoïdale à base elliptique dans un cristal cubique sous sollicitations extérieures arbitraires – III. Application aux systèmes de fissuration de monocristaux de $CoSi_2$

Les systèmes de fissuration fragile (<112> {111}, <113> {110}, <411> {122}) observés dans des monocristaux de $CoSi_2$ ont été confrontés à l'analyse théorique de la première partie de cette étude. Ceux-ci correspondent à des maximas moyens locaux positifs $< G >$, où la quantité $< G >$ est la force d'extension de la fissure G par unité de longueur du front de fissure, moyennée

sur toutes les positions sur le front de fissure. Par conséquent, les systèmes de fissures à l'équilibre fournis par la théorie sont ceux observés expérimentalement. Les systèmes de maclage et de fissuration sont du type <112> {111} comme prévu. Il est entendu que les résultats ci-dessus sont obtenus dans le cadre de la théorie de l'élasticité linéaire intégrant les dislocations en tant que défauts cristallins et éléments de base dans le traitement mathématique de la fracture.

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

I - INTRODUCTION

In the first part of this study [1], we have considered a conoidal nucleus of crack (vertex O) within an infinitely extended cubic material, arbitrarily oriented (O; $x_j^{'}$) with respect to the laboratory reference frame (O; x_j); the latter indicates the directions x_j of the externally applied loads ***(Figure 1)***. The general loading corresponds to tension σ_{22}^{a} and shears σ_{21}^{a} and σ_{23}^{a} along x_2, x_1 and x_3, respectively, with associated induced normal Poisson's stresses $-\nu_A(j)\sigma_{22}^{a}$ along x_1 (j=1) and x_3 (j=3). The nucleus has been represented by a continuous distribution of infinitesimal elliptic dislocation loops. Equilibrium dislocation distributions, boundary front stresses and extension force G per unit length have been expressed. $O\,x_2^{'}$ is a symmetrical axis of the crack nuclei. 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 running position P_D ($x_1^{'}, x_2^{'}, x_3^{'}$) at the elevation h along the base is written with respect to (O; $x_j^{'}$) as

$$\overrightarrow{OP}_D = \begin{pmatrix} x_1^{'} = \rho\sin\phi \\ x_2^{'} = h = \rho_1\tan\theta \\ x_3^{'} = \rho\cos\phi \end{pmatrix};\ -\pi \le \phi \le \pi,\quad 0 \le \theta < \pi/2;$$

$$\rho^2 = \rho_1^2 / (\sin^2\phi + a_r^2\cos^2\phi)\,. \qquad (1)$$

The angle ϕ is between $O'x_3^{'}$ and $O'P_D$ as shown in ***Figure 1***. Angle θ is measured in $O\,x_1^{'}\,x_2^{'}$ between $\boldsymbol{P_D}$ ($\phi = \pi/2$) $\boldsymbol{O'}$ and $\boldsymbol{P_D}$ ($\phi = \pi/2$) $\boldsymbol{O}$ 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 1***. Additional angular parameters θ_0 and ϕ_0 (Euler's angles) are introduced that connect $\vec{x}_j$ to $\vec{x}_j^{'}$.

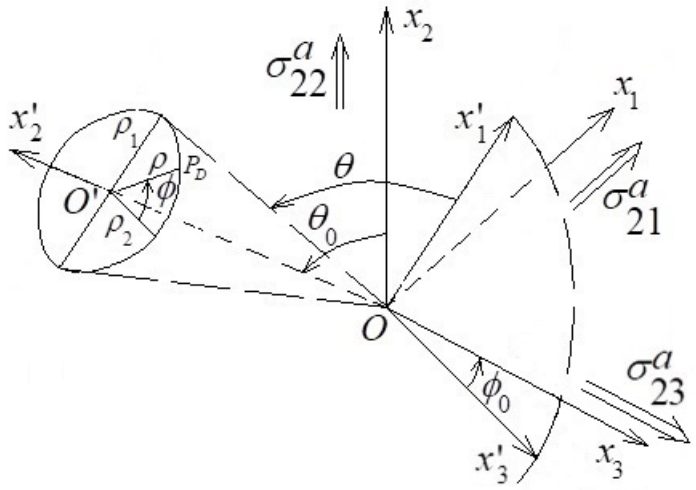

Figure 1 : *Elliptical base (elevation $x_2^{'} = OO' \equiv h$) of the conoidal crack with semiaxes ρ_1 and ρ_2 along $x_1^{'}$ and $x_3^{'}$. The running point P_D (1) along the base and angular parameters θ_0 and ϕ_0 that connect $\mathbf{x}_j$ and $\vec{x}_j^{'}$ are illustrated. Angle θ is introduced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

In the second part (*Part II*) of this study [2], the treatment in [1] with associated model ***(Figure 1)*** is applied to high temperature mechanical twinning systems *TS = [η_1] (K_1)* (η_1 and K_1 being the twinning direction and plane, respectively) observed in [112] copper single crystals deformed at constant strain rates. Primary close-packed twinning plane $(1\bar{1}1)$ = K_1*(a - c)* with associated twinning directions, η_1*(a)* = [121], η_1*(b)* = $[21\bar{1}]$ and η_1*(c)* = $[1\bar{1}\bar{2}]$, and the cross-slip $(11\bar{1})$ = K_1*(d)* plane with twinning direction η_1*(d)* = [112] ***(Figure 2)*** are considered. Graphical plots of $< G >$ as a function of θ_0 and ϕ_0, are displayed. Positive local $< G >$ maxima are observed for these twinning systems (except *TS(c)*) suggesting that these correspond to equilibrium configurations, in agreement with experiments. Equilibrium states during evolution are those observed over large time intervals and propagation

distances. In summary, 1/6 <112> {111} twinning corresponds to positive < *G* > maxima in copper. In this *part III*, the treatment in [1] with associated model ***(Figure 1)*** is used to find possible fracture systems *FS = [T] (F)* (*T* and *F* being the fracture direction and plane, respectively) in $CoSi_2$ single crystals. In *Section* 2, the methodology of the treatment is described. In *Section* 3, graphical representations of < *G* > are displayed corresponding to different fracture systems. *Section* 4 and 5 are devoted to discussion and conclusion, respectively.

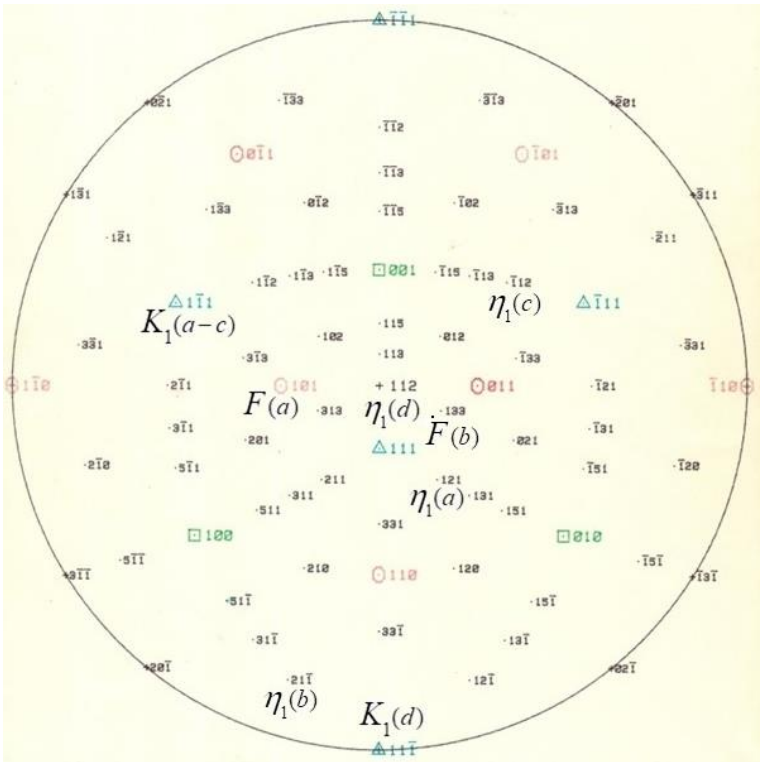

Figure 2 : *Stereographic projection with centre* [112] *for the identification of cracking and twinning systems*

II - METHODOLOGY

Figure 1 is used to specify a plane of fracture (*F*). x_2 is vertical, parallel to the applied tension, x_3 is then determined as the intersection between (*F*) 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 fracture systems under such conditions. Then graphical plots of < *G* > as a function of ϕ_0 are displayed. The crack propagation directions [*T*] in (*F*) are those associated to positive local maxima. It is assumed that the friction stresses are zero. The results for the {111} fractures are those of the twinning systems *TS(i)* mentioned earlier in

Section 1. Additional fracture planes (*F(j), j= a* and *b*) considered are:

(1) *F(a)* = (101): using ***Figures 1*** and ***2*** and indicating the directions only, we have $\theta_0 = 30°$, x_2 = [112], $x_3 = [11\bar{1}]$, $x_1 = [\bar{1}10]$, $x_2^{'} = [101]$

(2) *F(b)* = (122): $\theta_0 = 18°$, x_2 = [112], $x_3 = [\bar{4}02]$, $x_1 = [1\bar{5}2]$, $x_2^{'} = [122]$ (2)

For $CoSi_2$, C_{11} = 2.16, C_{12} = 1.35 and C_{44} = 0.81 in units of [10^{11} N / m^2], taken from [3]. $M_{12} = \sigma_{21}^a / \sigma_{22}^a$, $M_{13} = \sigma_{23}^a / \sigma_{22}^a$, $\nu_A(1) = \nu_A(3) = 1/3$, a_r = 4 / 3.

III - RESULTS

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

$$< \tilde{G} > = < G > / G_C^I = < \tilde{G} > (\theta, \theta_0, \phi_0, M_{12}, M_{13}, a_r, C_{nm}),$$

$$G_C^I = \frac{2^5 \alpha_0^2 a_r^4}{3\pi^2 C_{44}} (K_I^0)^2; \quad (3)$$

where $K_I^0 = \sigma_{22}^a \sqrt{\pi a_1}$. Octahedral fracture systems are invariably of the type < 112 > {111} as for the twinning systems and examples correspond to η_1[$a - d$] K_1 [$a - d$] of ***Figure 2*** [2]. Fracture plane *F(a)* = (101) is further considered and ***Figures 3*** and ***4*** are displayed in $CoSi_2$ material. Positive maxima of < $\tilde{G}$ > are at ϕ_0 = 60° and 10° approximately, respectively; these correspond to systems [$13\bar{1}$](101) and [$\bar{1}31$](101).

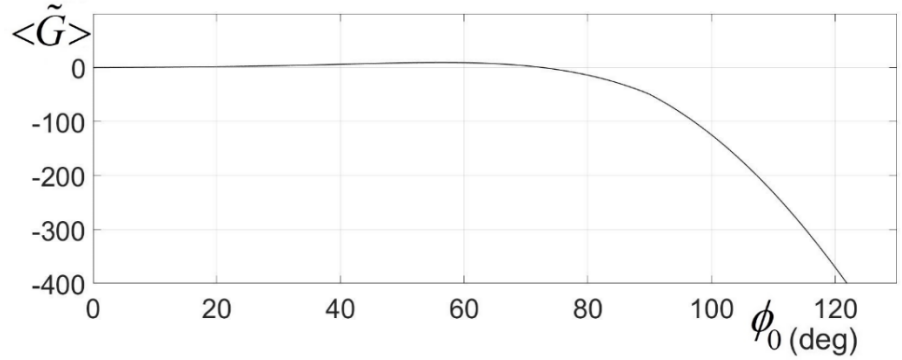

Figure 3 : < $\tilde{G}$ > (3) *as a function of* ϕ_0 *for* $\theta = \pi/3$ *and* θ_0 = 30°. *This corresponds to the fracture system* [$13\bar{1}$](101) (ϕ_0 = 60°). $M_{12} = M_{13} = 10^{-4}$, $\nu_A(1) = \nu_A(3) = 1/3$, a_r = 4 / 3, $CoSi_2$ *material.*

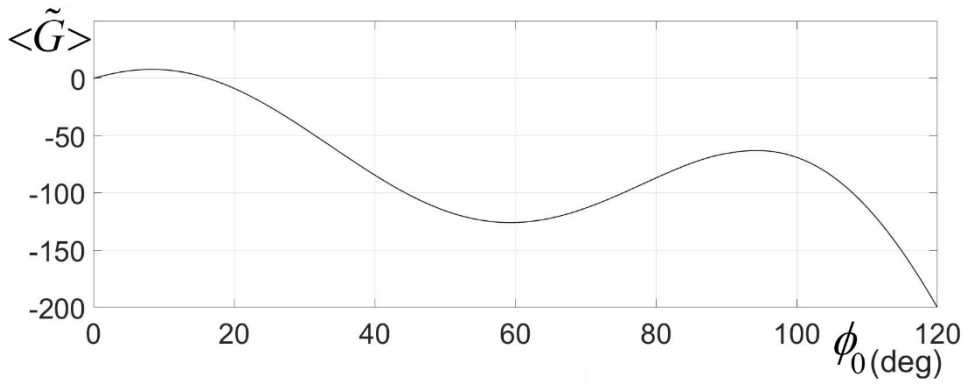

Figure 4 : $<\tilde{G}>$ *(3) as a function of* ϕ_0 *for* $\theta = \pi/3$ *and* $\theta_0 = 30°$*. This corresponds to the fracture system* $[\bar{1}31](101)$ *(*$\phi_0 = 10°$*).* $M_{12} = 1$, $M_{13} = 10^{-4}$ $\nu_A(1) = \nu_A(3) = 1/3$, a_r *= 4 / 3, CoSi₂ material.*

Consideration is also given to the fracture plane (122) = *F(b)* ***(Figures 5 and 6)***. Positive maxima of $<\tilde{G}>$ are at ϕ_0 = 50° and 110°, corresponding to $[\bar{2}\bar{2}3](122)$ and $[\bar{4}11](122)$, respectively.

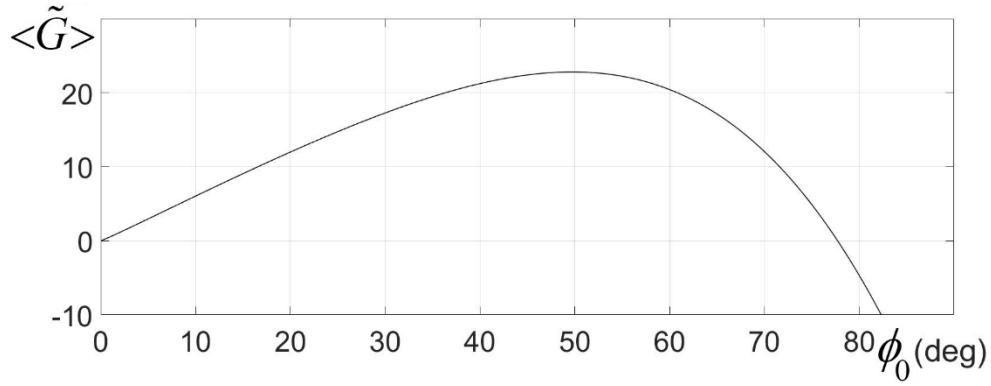

Figure 5 : $<\tilde{G}>$ *(3) as a function of* ϕ_0 *for* $\theta = \pi/3$ *and* $\theta_0 = 18°$*. This corresponds to the fracture system* $[\bar{2}\bar{2}3](122)$ *(*$\phi_0 = 50°$*).* $M_{12} = M_{13} = 10^{-4}$, $\nu_A(1) = \nu_A(3) = 1/3$, a_r *= 4 / 3, CoSi₂ material.*

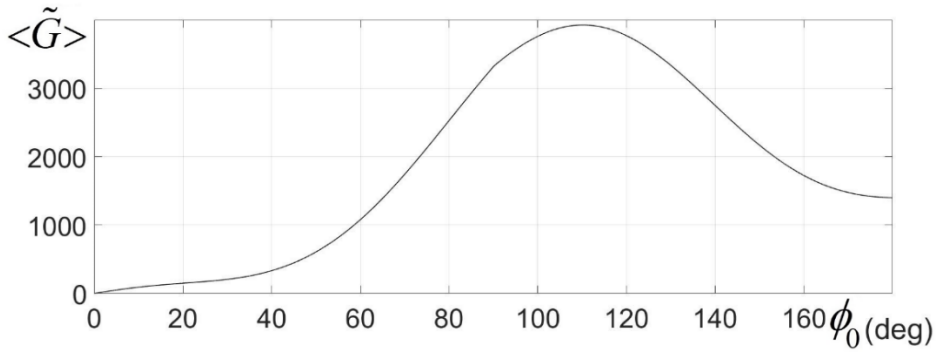

Figure 6 : $< \tilde{G} >$ (3) *as a function of* ϕ_0 *for* $\theta = \pi / 3$ *and* $\theta_0 = 18°$. *This corresponds to the fracture system* $[\bar{4}11](122)$ *(*$\phi_0 = 110°$*).* $M_{12} = 4$, $M_{13} = 10^{-4}$ $\nu_A(1) = \nu_A(3) = 1/3$, $a_r = 4/3$, $CoSi_2$ *material.*

It is stressed that < 110 > is not a fracture propagation direction in the fracture planes investigated. Also increasing the shearing stress M_{13} reduces $< \tilde{G} >$ to negative values; this means that this stress works against the expansion of the cracks.

IV - DISCUSSION

The experimental works on $CoSi_2$ [3 – 6] will serve for confrontation. Fractures on close-packed octahedral planes {111} have invariably a < 112 > propagation direction [4 – 6]. In [113] $CoSi_2$ single crystals deformed under compression up to brittle fracture, the fracture system is [112] $(11\bar{1})$ = $\eta_1(d)$ $K_1(d)$, ***Figure 2*** : this is clearly shown on the micrograph (see *Fig.* 2*a* of [5]). Agreement between theory and experiment is complete. Twinning and fracture systems are the same < 112 > {111}. The theory is describing twinning and fracture by representing these with continuous distributions of Volterra infinitesimal dislocations. Fractures on (101) [4, 6] suggest that the direction of fracture propagation is $[13\bar{1}]$ (see *Fig.*4 of [4] and *Table* 1 there for the numerous number of specimens involved). This is confirmed by the present analysis ***(Figure 3)***. Increasing the shearing stress M_{12} ***(Figure 4)*** provokes a change in the fracture propagation direction to $[\bar{1}31]$. Hence < 113 > seems the crack propagation direction in {101} planes. Fractures on (212) [4, 6] clearly indicate that the fracture propagation direction is $[\bar{1}4\bar{1}]$. ***Figure 6*** has predicted the cracking system $[\bar{4}11]$ (122) for sufficiently large M_{12} = 4. For small shearing stresses, ***Figure 5*** suggests the system $[\bar{2}\bar{2}3]$ (122). Increasing M_{13} works against crack expansion. This is because σ_{23}^{a} in the modelling ***(Figure 1)*** lies parallel to the elliptic crack front. This negative role has been mentioned earlier [7]. **V - CONCLUSION**

Brittle fracture systems (<112> {111}, <113> {110}, <411> {122}) observed in $CoSi_2$ single crystals [3 – 6] have been confronted to the theoretical analysis of Part I of this study [1]. These do correspond to positive local average $< G >$ maxima, where the quantity $< G >$ is the crack extension force G per unit length of the crack front, averaged other all the positions on the crack front. Hence, equilibrium crack systems provided by the theory are those observed experimentally. Both twinning [2] and cracking systems are of the type <112> {111} as expected. It is understood that above results are achieved within the framework of the theory of linear elasticity incorporating dislocations as crystal defects and basic elements in the mathematical treatment of fracture.

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