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**DILATATION FIELD OF A REGULAR
HEXAGONAL NETWORK OF MISFIT
DISLOCATIONS. APPLICATION TO (111) Si //
(111) CoSi₂**

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Introduction

Diffusion phenomena under stress control the movements of misfit dislocations at high temperatures, e.g., [1,2]. For a better understanding of the diffusion paths of vacancies and atomic species on each side of the interface, it is necessary to determine all the elastic dilatation field θ since these paths are orthonormal curves to equi-dilatation surfaces. In addition, elastic interactions between all linear interfacial defects must be taken into account for an accurate description of θ . A brief review of works involving the elastic fields of interfacial dislocations with a non planar deformation field shows in fact that no solutions exist yet in the literature for θ , even for the simplest case of a regular hexagonal network of misfit dislocations, which is in practise a common case observed in transmission electron microscopy, e.g., [3-6].

Since the first works [7,8] on low angle boundaries forming hexagonal patterns of dislocations lying parallel to (111) or (001) planes of cubic crystals, some authors have been faced with the problem of determining the stress fields and energies of dislocations visible along grain boundaries [9-12]. On the other hand, for a regular hexagonal pattern of misfit dislocations along an interphase boundary, the elastic field along the interface has not yet been obtained, except a formal solution derived from a double Fourier series analysis [13]. In this reference, to which the reader has to refer for notations, two different elastically isotropic media are used. The displacement field $\mathbf{u}$ is assumed to be biperiodic with two period vectors $\mathbf{OA}=\mathbf{a}$ and $\mathbf{OC}=\mathbf{c}$, as shown in Fig. 1, where O is the center of the hexagon UVWRSZU. However, only a formal result was presented because :

(i) the problem was found untractable for the most common case of any two media. Indeed, an algebraical inversion of a linear system of 12 equations with 12 unknowns, equ. (26) in [13], could not be achieved.

(ii) the non zero expressions of the right parts of the 12 above mentioned equations depend on the components of two undetermined vectors $\mathbf{H}^{(G)}$ and $\mathbf{T}^{(G)}$. These vectors are in fact depending on the geometry of the unit cell ($\mathbf{a}, \mathbf{c}$), the Burgers vectors of the dislocations, and the way to place the Cartesian frame $Ox_1x_2x_3$ relative to a hexagonal cell.

The aim of the present note is first to present a definitive answer for point (i), while for point (ii) and for the geometry of Fig. 1 the vectors $\mathbf{H}^{(G)}$ and $\mathbf{T}^{(G)}$ will be given. As a result, the complete displacement field can also be obtained. The volumic dilatation field will

be presented explicitly versus the geometrical parameters of a regular hexagonal network. A numerical application will be made for the volumic dilatation θ along the interphase boundary of a model system Si/CoSi₂ interface, which has been subjected to numerous investigations e.g. [5,14,15].

Explicit solutions for eq. (26) in ref. [13]

Let us first answer to point (ii) mentioned above, for convenience.

For simplification, the Cartesian frame $Ox_1x_2x_3$ described in [13] will be centered in O so that $\mathbf{H}(\mathbf{G})=0$, since the three components of the interfacial relative displacement are odd functions with x_1 and x_3 . The geometry of a regular hexagon UVWRSZ is characterized by

- two period vectors $\mathbf{a}$ and $\mathbf{c}$ making an angle $(\mathbf{a},\mathbf{c})$ equal to 60 degrees, with $|\mathbf{a}|=|\mathbf{c}|$.
- a point U such that $\mathbf{OU} = (\mathbf{a}+\mathbf{c})/3$.

The elastic field also depends on the Burgers vectors of the misfit dislocations. These latter have their lines oriented clockwise in Fig. 1. For practical purposes, only two of them need to be considered, our choice being the segments ZU and UV with Burgers vectors $\mathbf{b}(\text{zu})$ and $\mathbf{b}(\text{uv})$.

The vector $\mathbf{T}(\mathbf{G})$, with components (T_1, T_2, T_3) , has been obtained from cumbersome integrations [16]. It depends on the non-zero reciprocal vector $\mathbf{G}(m,n)$, where m, n are algebraic integers. The result is the following :

Figure 1 : A regular hexagonal network of misfit dislocations oriented clockwise UVWRSZ around the center O of a hexagon. $\mathbf{OA}$ and $\mathbf{OC}$ are the period vectors. The Cartesian frame used is $Ox_1x_2x_3$ with Ox_2 normal to the interface towards medium +, and $Ox_3 // \mathbf{OC}$. The angle $(\mathbf{OC}, \mathbf{OA})$ is 60 degrees.

for $m + n \neq 0$ and $n - 2m \neq 0$ and $m - 2n \neq 0$

$$\mathbf{T}^{(G)} = \frac{3 \sin \left[\frac{2\pi}{3} (m + n) \right]}{\pi^2 (m + n)} \left[\frac{\mathbf{b}^{(ZU)}}{n - 2m} + \frac{\mathbf{b}^{(UV)}}{m - 2n} \right] \quad (1)$$

for $m + n = 0$ and $m \neq 0$

$$\mathbf{T}^{(G)} = \frac{1}{3\pi m} [\mathbf{b}^{(ZU)} - \mathbf{b}^{(UV)}] \quad (2)$$

for $n - 2m = 0$ and $m + n \neq 0$

$$\mathbf{T}^{(G)} = \frac{(-1)^{(n+1)}}{\pi (m + n)} \mathbf{b}^{(ZU)} \quad (3)$$

for $m - 2n = 0$ and $m + n \neq 0$

$$\mathbf{T}^{(G)} = \frac{(-1)^{(m+1)}}{\pi (m + n)} \mathbf{b}^{(UV)} \quad (4)$$

The validity of these expressions has been checked numerically in computing, for some points inside the hexagon, the interfacial relative displacement of the crystals by two different ways : (i) from the limiting boundary condition (linear variation with x_1 and x_3); (ii) from the sum of the double Fourier series involving the $\mathbf{T}^{(G)}$'s.

Let us now turn to point (i). In eqs. (26) of [13], the unknowns are A_i and B_i ($i=1,2,3$), for each crystal + or -. In passing, let us correct a misprint in the 12th eqs. (26) : the term B_3^- must be changed into B_1^- . The unknowns have been derived explicitly from the solution of the 12 linear equations, thanks to a formal algebra software :

$$A_1^+ = sG_1 T_2 / (G\Delta) \quad A_1^- = A_1^+ \quad (5)$$

$$A_2^+ = -T_2 / \left[\left(\frac{1}{k} + 3 - 4v^+ \right) \right] \quad A_2^- = -T_2 / [k + 3 - 4v^-] \quad (6)$$

$$A_3^+ = sG_3 T_2 / (G\Delta) \quad A_3^- = A_3^+ \quad (7)$$

$$B_1^+ = - (p G_3^2 T_1 + q G_1 G_3 T_3 + r G_1^2 T_1) / (G^2 \Delta) \quad B_1^- = - B_1^+ - T_1 \quad (8)$$

$$B_2^+ = (G_1 T_1 + G_3 T_3) / \left[G \left(\frac{1}{k} + 3 - 4v^+ \right) \right] \quad B_2^- = (G_1 T_1 + G_3 T_3) / [G (k + 3 - 4v^-)] \quad (9)$$

$$B_3^+ = - (p G_1^2 T_3 + q G_1 G_3 T_1 + r G_3^2 T_3) / (G^2 \Delta) \quad B_3^- = - B_3^+ - T_3 \quad (10)$$

$$\text{where} \quad k = \mu^- / \mu^+ \quad (11)$$

$$p = k (3 + k - 4v^-) [1 + k (3 - 4v^+)] \quad (12)$$

$$q = 2k [1 - v^- - 3v^+ + 4v^- v^+ + k (-1 + 3v^- + v^+ - 4v^- v^+)] \quad (13)$$

$$r = k (1 + k) [5 - 6v^- - 6v^+ + 8v^- v^+ + k (3 - 4v^+)] \quad (14)$$

$$s = 2k(1+k)(2 - 3v^- - 3v^+ + 4v^-v^+) \quad (15)$$

$$\Delta = (1+k)(3+k-4v^-)[1+k(3-4v^+)] = p(1+k)/k \quad (16)$$

The above solutions for A_i and B_i ($i=1,2,3$) have been reinserted into the 12×12 system for the 12 equalities to be checked algebraically. Note that expressions (5-16) are valid whatever be the geometry of the hexagonal network, while expressions (1-4) are only specific to Fig. 1.

The dilatation field surrounding a regular hexagonal network of misfit dislocations

The dilatation field is defined by the classical formula [17]:

$$\theta = \frac{\partial u_1}{\partial x_1} + \frac{\partial u_2}{\partial x_2} + \frac{\partial u_3}{\partial x_3} \quad (17)$$

The derivatives are calculated from the expressions of the displacements [13] in which the A_i and B_i 's to be used are given, for each medium, by our expressions (1-16). The result shows that, for a given medium, θ only depends on the ratio k and on the Poisson's coefficient of the medium. Putting the convenient superscript + or - to appropriate symbols,

$$\theta = 4\pi(1-2v)\text{sign}(x_2) \sum_D G \{ B_2 \cos[2\pi(G_1x_1+G_3x_3)] + A_2 \sin[2\pi(G_1x_1+G_3x_3)] \} e^{-2\pi G|x_2|} \quad (18)$$

with $\text{sign}(x_2) = +1$ for medium +, and -1 for medium -. Series (18) converges for non zero x_2 , because of the exponential term. However, just at the interface ($x_2=0$), the series diverges because of an interfacial discontinuity of θ .

Series (18) becomes more simple if the Burgers vectors are parallel to the interface. In this case, if the edge and screw components of the dislocation segment UV are respectively denoted b_e and b_s , the components of the Burgers vectors involved in expressions (1-4) are

$$\mathbf{b}(zu) = 1/2 [(b_s + b_e \sqrt{3}), 0, (-b_s \sqrt{3} + b_e)] \quad \text{and} \quad \mathbf{b}(uv) = [b_s, 0, b_e] \quad (19)$$

then $T_2 = 0$ and consequently $A_2 = 0$. As a result, for medium +

$$\theta^+ = \frac{4\pi(1-2v^+)}{\left(\frac{1}{k} + 3 - 4v^+\right)} \sum_D \{ (G_1T_1 + G_3T_3) \cos[2\pi(G_1x_1+G_3x_3)] \} e^{-2\pi Gx_2} \quad (20)$$

The same formula applies to medium -, except some minor changes (v^+ into v^- ; $1/k$ into k ; 4π into -4π ; $-2\pi G$ into $+2\pi G$).

Only the dilatation field θ towards $x_2 > 0$ needs to be computed. θ^- in $(x_1, -x_2, x_3)$ is readily derived from θ^+ in the point (x_1, x_2, x_3) , since

$$\theta^- = - \frac{\mu^- (1 - 2\nu^-) [\mu^- + \mu^+ (3 - 4\nu^+)]}{\mu^+ (1 - 2\nu^+) [\mu^+ + \mu^- (3 - 4\nu^-)]} \theta^+ \quad (21)$$

As a result, for a grain boundary, the dilatation is an odd function with x_2 .

Application to Si/CoSi₂

Formula (20) has been applied to the regular hexagonal network of $1/6\langle 112 \rangle$ Si edge misfit dislocations as observed in [5] for the interface Si/CoSi₂, in order to have a quantitative idea of the change in the dilatation on either side of the interface.

The orientation relationship of both crystals is the "heterotwin" orientation [5], for which (111)CoSi₂/(111)Si. The silicon is chosen towards $x_2 > 0$. The data are the following :

lattice parameters [18]: Si = 0.54309 nm ; CoSi₂ = 0.5356 nm ; $b_e = -0.2217$ nm ; $b_s = 0$.
misfit $\epsilon = 0.0145$; the periods $|a| = |c|$ were calculated as equal to $|b_e|/\epsilon = 15.6$ nm.

The elastic constants were computed following Appendix 2 of [19], from anisotropic C_{ij} given in [17] for Si, [20] for CoSi₂ :

$$\mu^+ (\text{Si}) = 6.611 \cdot 10^{10} \text{ Pa} ; \nu^+ = 0.23.$$

$$\mu^- (\text{CoSi}_2) = 6.402 \cdot 10^{10} \text{ Pa} ; \nu^- = 0.34.$$

A FORTRAN programme was written to compute the variations of θ versus x_2 in each medium + (Si) and - (CoSi₂), when the running point is (i) along Ox_2 ; curve 2 in Fig. 2; (ii) along a line parallel to Ox_2 and passing through a triple node Z ; curve 1 in Fig. 2. On the curves 1 and 2, only the open and filled dots were computed. The summation parameters m and n were risen up to 60 for good convergence of the double Fourier series. For the two curves, θ tends to practically zero at distances close to one period. Around the center O of a hexagon, and as expected from the lattice parameters, Si appears to be in tension and the

Figure 2 : Change of the elastic dilatation θ in the vicinity of the interface Si/CoSi₂ with the distance x_2 to the boundary. Curve 1 : θ is varying from a triple node of the hexagonal network of dislocations. Curve 2 : θ is varying from the centre of a hexagon.

other phase in compression. Close to the triple node Z the situation is reverse, θ diverging for $x_2=0$. Note the large discontinuity of θ across the interface around O (about 0.016) and the large θ gradient along the interface. Around O, its value is obtained from an extrapolation of the two part of curves 2 for $x_2=0$. Relation (21) is here $\theta^- = -0.676 \theta^+$, which is valid except for $x_2=0$.

Summary

The displacement field of any regular hexagonal pattern of misfit dislocations has been thoroughly expressed from an analytical solution of a system of 12×12 linear equations given in [13]. The dilatation field θ induced by such a network has been derived explicitly under the form of a double Fourier series. For a grain boundary θ is an odd function with the coordinate x_2 perpendicular to the interface whatever be the Burgers vectors. The solution has been applied to the case of an observed misfit dislocation network on the (111)CoSi₂/(111)Si interface. Strong discontinuities of θ can be observed when crossing, or along, the interface.

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