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Elasticity theory of straight dislocations in a multilayer

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The question of describing the displacement and stress fields associated with straight misfit dislocations (MD's) located in a multilayer involving any N heterointerfaces or free surfaces is reduced, as well as other related problems, to the inversion of two independent sets of linear equations. The displacement field **u** of a single translation dislocation (TD) is obtained as the limit of an infinite spacing between two MD's. The multilayer can be limited by one or two free surfaces (epitaxy, thin foils). The simplicity and the power of the method is illustrated in solving classical but yet unsolved questions: the stress field associated with an edge interfacial TD in a layer sandwiched between two semi-infinite media ($N=2$), the **u** fields of two different interfacial edge TD's in a thin bicrystal ($N=3$), and the stress field associated with a multilayer formed by alternating GaAs and Si layers ($N=5$) containing a single array of edge MD's along one of the heterointerfaces.

I. INTRODUCTION

Since the theoretical work by Koehler,[1] who proposed to build multilayers made of ultrathin lamellae to improve the mechanical properties of composite materials, some experimental studies have confirmed that almost perfect thin multilayers can be prepared so as to obtain higher yield strengths relative to their bulk constituents, as well as higher ductility and toughness, e.g., Refs. 2 and 3. These exceptional properties are mainly due to an increased resistance to dislocation motion produced by image forces from nearby heterointerfaces. On the other hand, heterostructures which produce better efficiency for optoelectronic devices involve the formation of interfacial defects[4–7] and hence image force effects.

For this class of heterogeneous materials, the elastic properties of the dislocations are presently difficult to describe. To date, no exact theory is available to solve the following fundamental problem: What is the displacement and stress field of a straight dislocation parallel to the interfaces of a laminated medium containing N interfaces, among which possible free surface(s)? The difficulty is revealed by the number of accumulated attempts to only face the cases $N=1,2,3$, cf. Refs. 8–23: (i) a bicrystal without free surface, (ii) with one free surface, i.e., an epitaxial layer on a substrate, (iii) with two free surfaces, i.e., a bicrystalline foil. Very few works deal with the cases $N=3$ or 4,[22,24,25] and only concern screw dislocations. In Refs. 8–23, different mathematical methods were used, based either on the properties of harmonic functions, the superposition of particular two-dimensional problems, surface virtual dislocations, or, more commonly, image dislocations.

Below, a global approach is developed, based on the properties of the differential equations of elasticity for periodic solutions. It proves to be particularly powerful since the displacement field **u** can be computed for any N values. The stress field is then derived from derivation and application of the Hooke law. In addition, the approach can account for the particular positions of the heterointerfaces and the isotropic elasticity constants of each layer.

II. THEORY

Three kinds of problems are described below (see Fig. 1). The axis Ox_1 of a Cartesian frame runs along the lower interface and Ox_2 is the common upwards normal to the heterointerfaces. The multilayer only contains an array of periodic misfit dislocations (MD's) with Burgers vector **b** (b_1,b_2,b_3), located at the particular interface $x_2=h_n$ which separates medium n and $(n+1)$. The period vector Λ is parallel to this interface and, consequently, the displacement field in each layer is periodic with Λ. One of the MD's is placed at $x_1=0$.

(i) The multilayer is built with a package of $(N-1)$ thin welded layers, sandwiched between two semi-infinite media denoted 1 and $(N+1)$. For the running layer j ($j=1$ to $N+1$), the elastic constants are (μ_j,ν_j). Each interface of index j separating medium j and $(j+1)$ is located at the height $x_2=h_j$.

(ii) The multilayer is as described in (i), but now has an upper free surface for $x_2=h_N$. There is no medium $(N+1)$.

(iii) The multilayer is as described in (i), but now has two

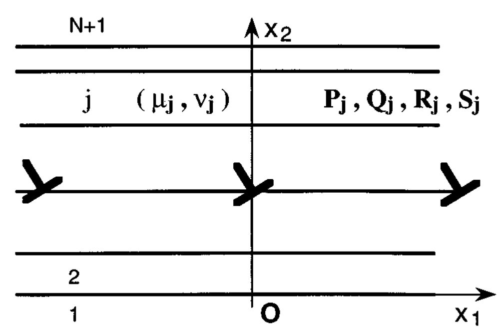

FIG. 1. Conventions and symbols describing an array of misfit dislocations in a multilayer with N heterointerfaces and $(N+1)$ media.

free surfaces for $x_2=h_1=0$ and for $x_2=h_N$. There are no media 1 and $(N+1)$.

From solutions of problems (i)–(iii), solutions of other related problems are immediately derived, e.g., those for which the MD's are slightly off the heterointerface in an infinite bicrystal,[11] in which case the MD network is considered as located along a fictitious interface separating two identical media $(N=2)$. Another case corresponds to a very large Λ [in comparison with the length separating the two more distant interfaces or free surface(s)], transforming the elastic field around a MD into that of a single translation dislocation (TD).

Let us now detail the boundary conditions of problems (i)–(iii), and express the route to obtain the displacement field u_k $(k=1,2,3)$. For all the solid–solid interfaces, the transmission of the forces is assumed. For a free surface, no stress is applied. Transmission of the **u** field is also assumed, except for the particular interface of index n. For this interface, along which lies the MD array $(x_2=h_n)$, the accommodation of the misfit is required and, hence, u_k is constrained to accommodate the misfit. This latter point merits special attention. As described in Ref. 10 and experimentally verified at a near-atomic scale in Refs. 7 and 26, this condition requires, along $x_2=h_n$, first, a sawtooth change of $\Delta u_k=[u_k^{(n+1)}-u_k^{(n)}]$; second, $\Delta u_k=0$ in the middle point between two MD's. (In Ref. 26, the first line of Eq. (4) must read $K^+=K^-=[1-L^-(3-4\nu^-)-L^+(3-4\nu^+)]/2.$) In terms of a continuous distribution of infinitesimal dislocations over a period Λ, the net Burgers vector is zero and long-range stresses are also zero. These imposed conditions reflect the presence of atomic structural units repeating along the interface via a gradual elastic deformation due to the preservation of the atomic neighbors despite the misfit between the lattices.[7,26,29]

The general expression of u_k as a complex Fourier series versus the coordinate x_1 of the Cartesian frame $Ox_1x_2x_3$ will now be written. Inside a layer of index j, the displacement field can then be expressed, with $\omega=2\pi/\Lambda$ and i as the square root of -1,

$$u_k^{(j)}=\sum_{-\infty}^{\infty} U_k^{(j,m)}e^{im\omega x_1}. \tag{1}$$

The three functions $U_k^{(j,m)}$ only depend on x_2. They are found explicitly in two steps: first, from the insertion of (1) into the differential equations of elasticity which leads to a system of three differential equations involving the three functions $U_k^{(j,m)}$ and, second, from the solutions of this system, as partly described in Ref. 10. Dropping the superscript (j,m) for simplicity, these solutions are

$$U_1=(P+Qm\omega x_2)e^{-m\omega x_2}+(R+Sm\omega x_2)e^{m\omega x_2}, \tag{2}$$

$$U_2=i[P+Q(3-4\nu)+Qm\omega x_2]e^{-m\omega x_2}-i[R-S(3-4\nu)+Sm\omega x_2]e^{m\omega x_2}, \tag{3}$$

$$U_3=Te^{-m\omega x_2}+Ue^{m\omega x_2}, \tag{4}$$

where P, Q, R, S, T, and U are coefficients depending only on the boundary conditions specified for problem (i), (ii), or (iii). In the following, the interface of index j separates the two consecutive layers, j and $(j+1)$. The boundary conditions in displacement concerning the particular interface along which lies the MD array $(x_2=h_n)$ are such that[10]

$$u_k^{(n+1)}-u_k^{(n)}=\sum_{-\infty}^{\infty}\frac{ib_k}{2\pi m}e^{im\omega x_1} \quad (m\neq 0). \tag{5}$$

Now, the boundary conditions in displacements and stresses attached to any given interface of index $j(1\leqslant j\leqslant N)$ can be expressed as the following six equations:

$$(\mathrm{I})\begin{cases} P_{(j+1)}/e_j+h_jQ_{(j+1)}/e_j+e_jR_{(j+1)}+e_jh_jS_{(j+1)}-P_j/e_j-h_jQ_j/e_i-e_jR_j-e_jh_jS_j=\delta_{jn}ib_1/(2m\pi), & (6)\\ P_{(j+1)}/e_j+(3+h_j-4\nu_{(j+1)})Q_{(j+1)}/e_j-e_jR_{(j+1)}+e_j(3-h_j-4\nu_{(j+1)})S_{(j+1)}-P_j/e_j+(-3-h_j+4\nu_j)Q_j/e_j+e_jR_j & \\ \quad +e_j(-3+h_j+4\nu_j)S_j=\delta_{jn}b_2/(2m\pi), & (7)\\ -s_jP_{(j+1)}/e_j+s_j(-2-h_j+2\nu_{(j+1)})Q_{(j+1)}/e_j-e_js_jR_{(j+1)}+e_js_j(2-h_j-2\nu_{(j+1)})S_{j+1}+P_j/e_j & \\ \quad +(2+h_j-2\nu_j)Q_j/e_j+e_jR_j+e_j(-2+h_j+2\nu_j)S_j=0, & (8)\\ s_jP_{(j+1)}/e_j+s_j(1+h_j-2\nu_{(j+1)})Q_{(j+1)}/e_j-e_js_jR_{(j+1)}+e_js_j(1-h_j-2\nu_{(j+1)})S_{(j+1)}-P_j/e_j & \\ \quad +(-1-h_j+2\nu_j)Q_j/e_j+e_jR_j+e_j(-1+h_j+2\nu_j)S_j=0, & (9)\end{cases}$$

$$(\mathrm{II})\begin{cases} T_{(j+1)}/e_j+e_jU_{(j+1)}-T_j/e_j-e_jU_j=\delta_{jn}b_3/(2m\pi), & (10)\\ T_{(j+1)}/e_j+e_js_jU_{(j+1)}-s_jT_j/e_j-e_jU_j=0, & (11)\end{cases}$$

where δ_{jn} is the Kronecker symbol, $e_j=\exp(m\omega h_j)$, and $s_j=\mu_{(j+1)}/\mu_j$.

Finally, the complete set of boundary conditions relative to all the N interfaces [including possible free surface(s)] are expressed in repeating Eqs. (6)–(11) for $j=1$ to N. The nonzero second members of the equations only appear for $j=n$. From the consideration of the independent systems (I) and (II) formed by Eqs. (6)–(9) and (10) and (11), it is concluded that the edge and screw components of the MD's have independent effects on the elastic field.

For problem (i), the convergence of the stress field in the two semi-infinite media 1 and $(N+1)$ requires $R=S=U=0$ for the medium $(N+1)$ and $P=Q=T=0$ for medium 1. The MD array can be located on any heterointerface of index n $(1 \leqslant n \leqslant N)$. As a result, a system of $6N$ linear equations with $6N$ unknowns has to be solved (denoted $6N \cdot 6N$). Note that this system split into two smaller independent systems: $4N \cdot 4N$ (edge component) and $2N \cdot 2N$ (screw component). For problem (ii), there is no upper medium, and the MD array can be located on any heterointerface of index n such that $1 \leqslant n < N$. But the convergence in the lower medium requires $P=Q=T=0$ for medium 1. Two smaller independent systems, $(4N-2)\cdot(4N-2)$ (edge component) and $(2N-1)\cdot(2N-1)$, have to be solved. For problem (iii), there is no semi-infinite media 1 and $(N+1)$, and the MD array can be located on any heterointerface of index n, such that $1 < n < N$. The number of heterointerfaces separating the thin layers is $(N-2)$. Two independent systems, $(4N-4)\cdot(4N-4)$ and $(2N-2)\cdot(2N-2)$, have to be solved.

III. APPLICATIONS

To illustrate the power of this approach, three numerical applications have been performed using a FORTRAN program, with $N=2$, 3, and 5.

The first example is related to the problem of a $Al/Al_2Cu(\theta)$ thin bicrystal containing an edge interfacial TD, i.e., problem (iii) with $N=3$ and two free surfaces. If the method of surface virtual dislocations can derive the stress field,[22] it does not yield easily to the displacement field **u**. Two kinds of Burgers vectors **b** are considered, perpendicular to the interface [Fig. 2(a)] or parallel [Fig. 2(b)]. These figures depict both the initial undeformed state (the three horizontal lines) and the surrounding two-dimensional (2D) displacement fields. The isotropic elasticity constants of the crystals were calculated from the anisotropic elastic constants given in Refs. 30 and 31 for Al and θ, according to an averaging method described in the Appendix of Ref. 32. Results are $\mu_{Al}=26.5$ GPa, $\nu_{Al}=0.347$, and $\mu_\theta=40.46$ GPa, $\nu_\theta=0.31$. Other data are the following: thicknesses of the two layers 5 nm (θ) and 2.5 nm (Al); lattice parameter for Al, $a_{Al}=0.4045$ nm.[33] In the Cartesian frame used, $Ox_1 \parallel [010]$Al and $Ox_2 \parallel [001]$Al, **b** is 1/2[101]Al for Fig. 2(a) and 1/2[110]Al for Fig. 2(b). The period Λ has been taken as ten times the total thickness of the bicrystal, i.e., 7.5 nm. These **u** fields generate the free surface curvatures and, around the dislocation cores, the deformations of lattices of pseudosquares of black points (θ below) or small black crosses (Al above). In the initial states, these points are separated by a spacing equal to 0.5 nm, and the two lattices of crosses and points are continuous. The displacement fields of the crystals are exaggerated by a factor of 3 for a better visual representation. Along the heterointerfaces, the lattices formed by the crosses and points are discontinuous, as expected for a translation dislocation.

The second example deals with the dislocated sandwich problem ($N=2$, no free surfaces), solved by Chou for a screw translation dislocation.[18] The sandwich is described in Fig. 3 by $Al/Al_2Cu(\theta)/Al$, $\mathbf{b}=1/2[011]\mathrm{Al} \parallel Ox_2$, and a thickness h of the θ crystal equal to 2 nm. Figure 3 illustrates the equistress curves $\sigma_{11}=\pm 30\times 10^7$ Pa obtained from the numerical solution of Eqs. (5)–(8). These curves stop abruptly at the upper heterointerface due to discontinuity in the σ_{11} field. The nonsymmetry of the curves relatively to the plane $x_2=0$ is due to a composite effect of the sandwich, since for a homogeneous medium, the symmetry is observed.[30] As for the first example, the ratio Λ/h was taken equal to 10 for these calculations (instead of infinity).

The third example is a multilayer with $N=5$, formed by four thin alternating GaAs and Si layers sandwiched between two semi-infinite media GaAs and Si. The choice of this heterostructure results from the number of works presented

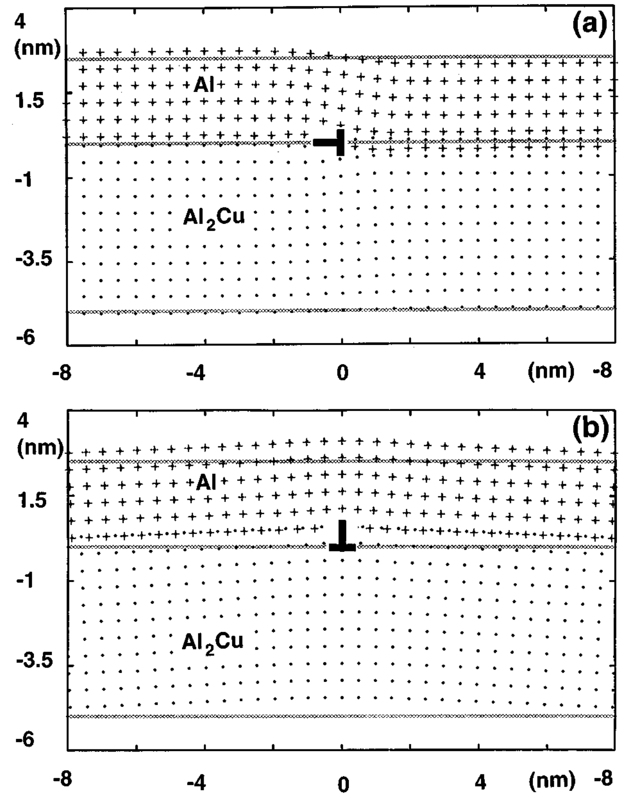

FIG. 2. $N=3$. Displacement fields in thin bicrystalline foils Al/Al_2Cu due to an edge interfacial dislocation. The **u** field is three times larger for convenience. The free surfaces and the nondeformed heterointerface are represented by the three horizontal lines at level -5, 0, and 2.5 nm. **b** is normal (a) or parallel (b) to the heterointerface.

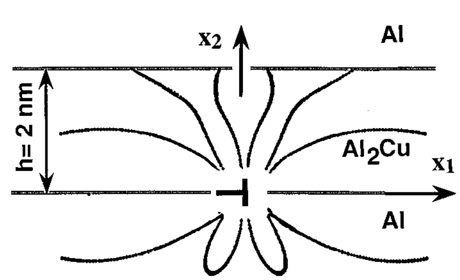

FIG. 3. $N=2$. An Al_2Cu layer is sandwiched between two semi-infinite Al crystals. Equistress curves $\sigma_{11}=\pm 30\times 10^7$ Pa corresponding to an edge dislocation perpendicular to the heterointerface.

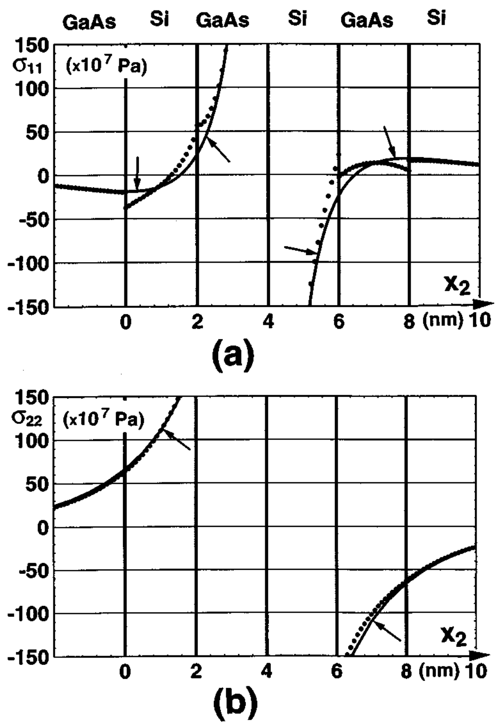

FIG. 4. $N=5$. Heterogeneous multilayer material formed by alternating six media GaAs and Si. The misfit dislocation array lies at $x_2=4$ nm. Changes of the (a) σ_{11} stress and (b) σ_{22} stress, along $x_1=0$ (see Fig. 1). In a homogeneous material with averaged elastic constants, these stresses are continuous (curves marked by thin arrows).

in the literature on these materials, e.g., Refs. 5–7. In this example, the intensities of the normal stresses have been evaluated along the axis Ox_2, as described in the Cartesian frame, shown in Fig. 1. The five heterointerfaces are located at (in nm) $x_2=0,2,4,6,8$. In Figs. 4(a) and 4(b), their positions are marked by the thick vertical lines. A single array of edge MD's with $\mathbf{b}=1/2\langle 110\rangle \mathrm{Si} \parallel Ox_1$ is assumed to be located along the interface $x_2=4$ nm. From the lattice parameters of GaAs [0.5653 nm (Ref. 34)] and Si [0.4045 nm (Ref. 33)], the length misfit is 4%, and the corresponding period Λ is 9.7 nm. On the other hand, $b_1=0.3838$ nm, $b_2=b_3=0$. The isotropic elasticity constants of the two crystals have been calculated from the anisotropic elasticity constants given in Refs. 30 and 35 and the procedure indicated in the appendix of Ref. 32. As a result, the isotropic constants are $\mu_{\mathrm{GaAs}}=46.01$ GPa, $\nu_{\mathrm{GaAs}}=0.24$, $\mu_{\mathrm{Si}}=66.11$ GPa, $\nu_{\mathrm{Si}}=0.23$. Figures 4(a) and 4(b) show curves which give an idea of the changes of the stresses σ_{11} and σ_{22} (curves in black dots) close to the MD core($x_2=d=4$ nm), where they diverge. The σ_{11} stress curve shows noticeable discontinuities when crossing the heterointerfaces at (in nm) $x_2=0,2,6,8$, conversely to the σ_{22} stress curve which remains continuous.

To appreciate the stress redistribution effect in the multilayer, the same calculations have been performed but for an elastically homogeneous medium with average μ and ν values. In this particular case, the stresses can be derived analytically from the two first expressions (32b) in Ref. 10 in which $q=1$. The result is

$$\sigma_{11}=2\mu\left(\frac{b_1}{\Lambda^2}\right)[\pi(x_2-d)F_3-\Lambda F_1 \mathrm{sgn}(x_2-d)]/(1-\nu), \tag{12}$$

$$\sigma_{22}=2\pi\mu(b_1/\Lambda^2)(x_2-d)F_3/(-1+\nu), \tag{13}$$

in which

$$F_1=\{([\sinh(\omega|x_2-d|)]/\phi)-1\}/2, \tag{14}$$

$$F_3=-[1-\cosh(\omega|x_2-d|)\cos(\omega x_1)]/(2\phi^2), \tag{15}$$

$$\phi=\cosh(\omega|x_2-d|)-\cos(\omega x_1), \tag{16}$$

$\mathrm{sgn}(x_2-d)=-1$ or $+1$, according to $(x_2-d)<0$ or >0, respectively.

For a period Λ tending to infinity, Eqs. (12) and (13) lead to the well-known σ_{11} and σ_{22} expressions of a single TD, see Ref. 30. For $\Lambda=9.7$ nm, Eqs. (12) and (13) lead to the continuous curves indicated in Fig. 4(a) by small arrows. In the middles of the layers 2 and 5, these curves cut the curves in black dots. However, close to the heterointerfaces of indices 1,2,4,5, the values obtained for σ_{11} are considerably different (see Table I). In contrast to these departures, the σ_{22} values are not sensitively different [see Fig. 4(b)].

IV. SUMMARY AND CONCLUSIONS

The displacement field $\mathbf{u}$ generated by a regular array of misfit dislocations MD's located in a multilayer material involving any number N of heterointerfaces or free surfaces, has been obtained in a Fourier series form from periodical solutions of the differential equations of elasticity. To respect the limiting boundary conditions along the N heterointerfaces, coupling equations between the Fourier series attached to each layer have to be established. With respect to the variety of methods presented in the literature[8–25] to cope with interface problems for $N=1,2,3,4$, see Refs. 8–25, the

TABLE I. σ_{11} values in a multilayer GaAs/Si with $N=5$. Heterointerfaces are located by x_2. Two assumptions are used: an elastically heterogeneous and of a homogeneous medium with averaged elastic constants. Note the strong σ_{11} discontinuities for the multilayer.

x_2 (in nm)	0	2	6	8
(multilayer) σ_{11} (in 10^7 Pa unit)	$-19.9/-37.7$	50.8/56.5	$23.0/-2.6$	4.7/16.1
(homogeneous medium) σ_{11} (in 10^7 Pa unit)	-18.8	23.6	-23.6	18.8

present approach treats all of these problems in a simple and global way. As examples of the power of the method, three very different and apparently unsolved problems have been treated, for $N=2$, 3, and 5; one of them involving two free surfaces $(N=3)$. For $N=5$, the multilayer is formed by alternating GaAs and Si crystals. Numerical results indicate a considerably redistribution of some stresses close to the heterointerfaces (see Table I), as compared to the assumption of an elastically homogeneous multilayer. With the present approach, any N value can be taken into consideration, as well as any thickness for each layer. The main limitation is the consuming time to invert the two sets of linear Eqs. (5)–(8) and (9) and (10). For the case of a unique TD, the $\mathbf{u}$ field is obtained at the limit of a large period Λ, before the total thickness of the multilayer. The numerical precision will depend on the number of harmonic terms retained in the calculation of the Fourier series and, consequently, numerical convergence tests are required. Finally, let us say that this approach also opens a new way to take account of the full anisotropic elasticity of the layers.

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