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ENERGY ANALYSIS OF DISLOCATION ARRAYS NEAR BIMATERIAL INTERFACES

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Abstract—Expressions for the elastic strain energies due to dislocation arrays near bimaterial interface or near the free surface of a semi-infinite body are derived. Arrays with periodic straight dislocations of edge, screw and combined type are considered. Expressions for the complete stress distribution and dislocation forces are also presented. © 1997 Elsevier Science Ltd. All rights reserved.

1. INTRODUCTION

Recently, a significant amount of research has been devoted to the evaluation of the elastic strain energy produced by dislocation arrays in various configurations relative to the free surface in a semi-infinite body or an interface in a multi-layer material (van der Merwe and Jesser, 1988; Willis *et al.*, 1990; 1991; Hirth and Feng, 1990; Freund; 1993, Gosling and Willis, 1994). The research was mainly motivated by the significance of energy expressions in the mechanics of semiconductor materials and the strain relaxation processes in thin films (Matthews, 1979; Jesser and van der Merwe, 1989; Freund, 1993). A study of the elastic strain energy and the stress fields produced by periodic dislocation arrays is also of importance in grain boundary modeling, analysis of polygonalization, persistent slip bands and dislocation cell structures (Nakahara *et al.*, 1972; Rey and Saada, 1975; Chou and Lin, 1975; Chou *et al.*, 1975; Hirth *et al.*, 1979; Saada, 1979; Hirth and Lothe, 1982; Lubarda *et al.*, 1993; Saada and Bouchand, 1993; Lubarda and Kouris, 1996a,b).

In this paper expressions for the elastic strain energy are derived due to infinite dislocation arrays parallel to the interface of two joined semi-infinite elastic bodies with different elastic constants. Section 2 is an analysis of an isolated dislocation near the bimaterial interface. In Section 3 the arrays with periodically distributed dislocations are considered. The arrays consist of screw dislocations, or edge dislocations whose Burgers vectors are either parallel or normal to the interface. A general dislocation array, consisting of mixed-type straight dislocations, is considered in Section 4. Expressions for the energy and dislocation forces are derived in each case. Results for the arrays near the free surface of a semi-infinite homogeneous body are also given. In the derivation process, a knowledge of the stress distribution produced by dislocations is needed. Expressions for all stress components produced by a single dislocation near the bimaterial interface are consequently listed in Appendix A. Appendix B presents the corresponding formulas for infinite dislocation arrays, which are obtained by appropriate summation from the formulas listed in Appendix A. In Appendix C we show that various energy contributions depend on a selected cut surface along which displacement discontinuity is imposed. Finally, in Appendix D we present an additional procedure to derive considered energy expressions.

2. SINGLE DISLOCATION NEAR A BIMATERIAL INTERFACE

Consider a general straight dislocation at a distance h from the interface of two joined isotropic elastic half spaces. The dislocation Burgers vector has the edge components, b_x and b_y, and the screw component, b_z. Let μ_1 and ν_1 be the shear modulus and Poisson ratio of material (1), and μ_2 and ν_2 of material (2). A complete adherence between two materials is assumed, so that displacements and tractions are continuous across the interface. The stress field for this problem was originally derived by Head (1953a,b), and further studied by Pastur *et al.* (1963), Dundurs (1969), and others. The relevant results for the purposes of this paper are listed in Appendix A. The following material parameters are conveniently utilized

$$k_1 = \frac{\mu_1}{2\pi(1-\nu_1)}, \quad k_2 = \frac{\alpha-\beta}{1+\beta}, \quad k_3 = \frac{1+\alpha}{1-\beta^2}, \quad k_4 = \frac{\mu_1-\mu_2}{\mu_1+\mu_2} \tag{1}$$

where α and β are the non-dimensional Dundurs parameters, defined by

$$\alpha = \frac{(1-\nu_1)\mu_2-(1-\nu_2)\mu_1}{(1-\nu_1)\mu_2+(1-\nu_2)\mu_1}, \quad 2\beta = \frac{(1-2\nu_1)\mu_2-(1-2\nu_2)\mu_1}{(1-\nu_1)\mu_2+(1-\nu_2)\mu_1}. \tag{2}$$

If the two materials are identical, $\alpha = \beta = 0$, $k_2 = k_4 = 0$, and $k_3 = 1$. Also, $k_3 - 1 = (\alpha+\beta^2)/(1-\beta^2)$, and $1+k_2 = (1-\beta)k_3$. The constants k_2 and k_3 are related to constants Q and M used by Pastur *et al.* (1963), and Chou and Lin (1975) through the relations $k_2 = -Q$ and $k_3 = -M/\beta$.

Since the elastic strain energy in the system does not depend on the vertical position of dislocation along the line $x = h$, the total force on a dislocation per unit length, exerted by the interface, is in the horizontal direction and given by $F_x = b_x\sigma_{xy}^{(1)}(h,0) + b_y\sigma_y^{(1)}(h,0) + b_z \sigma_{zy}^{(1)}(h,0)$. The divergent part of the stress at the core center of the dislocation is excluded in this expression. For example, for a pure edge dislocation with the Burgers vector normal to the interface, the (glide) force is $F_x = k_1(k_3-1)b_x^2/2h$, originally derived by Pastur *et al.* (1963). The nature of this force (attractive or repulsive toward the interface) depends on the combination of material properties α and β, and is discussed by Dundurs (1969). The tractions over any plane parallel to the interface have a non-vanishing resultant $\beta\pi k_1 k_3 b_x$, parallel to the interface. This was originally observed by Dundurs and Sendeckyj (1965), and later discussed by Comninou (1977), Barnett and Lothe (1974), Lothe (1992), and others.

The elastic strain energy per unit dislocation length within a large cylinder of radius $R \gg h$ around the dislocation, excluding its core, can be conveniently expressed by using the divergence theorem. For a pure edge dislocation with the Burgers vector b_x, the energy is

$$E = \frac{1}{2} b_x \int_{h+\rho}^{R} \sigma_{xy}^{(1)}(x,0)\,\mathrm{d}x + E_R - E_\rho, \tag{3}$$

where E_R is the contribution from the tractions at the remote contour of radius R, and E_ρ from the tractions at the dislocation core surface of radius ρ. Substitution of expression (A.11) from Appendix A for the shear stress $\sigma_{xy}^{(1)}(x,0)$ gives

$$E = \frac{1}{2} k_1 b_x^2 \left(\ln\frac{2h}{\rho} + k_3 \ln\frac{R}{2h} + \frac{k_2}{2} \right) + E_R - E_\rho. \tag{4}$$

For a sufficiently small core radius ($\rho \ll h$), the energy E_ρ can be calculated by replacing the dislocation core with a cylindrical hole, whose surface is subjected to tractions of an isolated dislocation in an infinite homogeneous medium, along with the corresponding displacements. When displacement discontinuity is imposed along the horizontal cut, this gives $E_\rho = k_1 b_x^2(1-2\nu_1)/8(1-\nu_1)$. The energy contribution E_R can be conveniently calculated by using the stress and displacement fields of an interfacial dislocation, since the distance h between the dislocation and interface is not observed at a far remote contour R. The relevant traction and displacement components for the interface dislocation can be found in Dundurs and Mura (1964), which upon integration gives

$$E_R = \frac{k_1 k_3 b_x^2}{8(1-\nu_1)}\left\{[2+(3-2\beta+\beta^2)(1-2\nu_1)]k_3 - 2\frac{(1+\beta)(2-\beta)}{1-\beta}(1-\nu_1)\right\}. \tag{5}$$

In the case of a uniform infinite medium ($\beta = 0, k_3 = 1$), E_R reduces to E_ρ, so that the core and remote contour contributions in eqn (4) cancel each other. If a dislocation is near the free surface of a semi-infinite body, the energy contribution from the remote contour vanishes, because the stresses decrease as $1/r^2$ far away from the dislocation. It is pointed out that, when using a divergence theorem to calculate elastic strain energy for a dislocation in an infinite bimaterial or in a semi-infinite homogeneous body, the individual energy contributions from the cut surface, remote contour and the core surface in general depend on the selected cut along which displacement discontinuity is imposed. However, the total elastic strain energy is independent of such a selection, since neither stress nor strain depend on the cut. This is discussed in more detail in Appendix C of this paper.

The elastic strain energy per unit length of a screw dislocation within a large cylinder of radius $R \gg h$ around the dislocation is

$$E = \frac{1}{2} b_z \int_{h+\rho}^{R} \sigma_{zy}^{(1)}(x,0)\,\mathrm{d}x. \tag{6}$$

There is no contribution from the tractions at the remote contour of radius R, since for an interface screw dislocation it follows that $\sigma_{zr} = 0$ (hence, no work is done on the u_z displacement). Similarly, there is no contribution from the tractions on the core surface for a screw dislocation in an infinite homogeneous body. In view of eqn (A.4), eqn (6) therefore gives

$$E = \frac{\mu_1 b_z^2}{4\pi}\left[(1-k_4)\ln\frac{R}{2h} + \ln\frac{2h}{\rho}\right]. \tag{7}$$

If $k_4 = 1$, the first term on the right-hand side of eqn (7) is equal to zero, and the strain energy for a screw dislocation near the free surface of a semi-infinite body is obtained.

Since there is no interaction term between the edge and screw dislocation contributions, the elastic strain energy of a general straight dislocation is the sum of the individual energy contributions. This gives

$$E = \frac{1}{2}k_1\left\{(b_x^2+b_y^2)\left(\ln\frac{2h}{\rho} + k_3\ln\frac{R}{2h} + \frac{k_2}{2}\right) + (1-\nu_1)b_z^2\left[\ln\frac{2h}{\rho} + (1-k_4)\ln\frac{R}{2h}\right]\right\} + E_R - E_\rho. \tag{8}$$

The corresponding dislocation force, the negative gradient of E with respect to h, is

$$F_x = -\frac{1}{2}k_1[(1-k_3)(b_x^2+b_y^2) + (1-\nu_1)k_4 b_z^2]\frac{1}{h}. \tag{9}$$

In eqn (8), E_R and E_ρ are the contributions from the tractions at the remote contour and the dislocation core surface. When displacement discontinuity is imposed along the horizontal cut, the energy contribution from the core surface is

$$E_\rho = \frac{1}{4}k_1\left[(b_x^2-b_y^2) - \frac{1}{2(1-\nu_1)}(b_x^2+b_y^2)\right]. \tag{10}$$

The elastic strain energy for a dislocation near the free surface of a semi-infinite body is

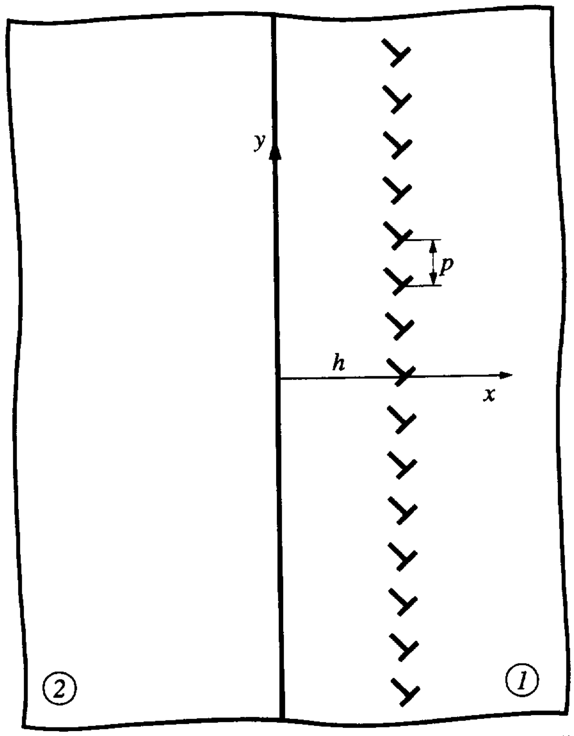

Fig. 1. A general dislocation array of uniform dislocation spacing p, at a distance h from the bimaterial interface.

obtained by inserting into eqn (8) $k_2 = -1$, $k_3 = 0$, $k_4 = 1$, $E_R = 0$, and by using eqn (10) for the core contribution E_ρ. The result is

$$E = \frac{1}{2}k_1\left\{[b_x^2+b_y^2+(1-\nu_1)b_z^2]\ln\frac{2h}{\rho} - \frac{1}{4(1-\nu_1)}[(3-4\nu_1)b_x^2-b_y^2]\right\}, \tag{11}$$

in agreement with Freund (1987, 1990).

3. DISLOCATION ARRAY NEAR A BIMATERIAL INTERFACE

Consider an infinitely long dislocation array at a distance h from the interface of two joined materials (Fig. 1). The array consists of identical, uniformly spaced dislocations of spacing p. The Burgers vectors of dislocations consist of the edge and screw components. The stresses at an arbitrary point are obtained by adding the contributions from all dislocations in the array. The summation procedure is rather lengthy. Chou and Lin (1975) gave implicit expressions for the stresses in material (1), in the case of edge dislocations with Burgers vectors normal to the interface. Stresses for other orientations of dislocations have apparently not been reported in the literature. We have consequently performed requisite summations and derived explicit expressions for all stress components in both materials, and for all three types of dislocation arrays. The results are listed in Appendix B. In these expressions the non-dimensional variables are used: $\xi = x/p$, $\eta = y/p$, $h_0 = h/p$, and $\vartheta = 2\pi(\xi - h_0)$, $\varphi = 2\pi(\xi + h_0)$, $\psi = 2\pi\eta$. The abbreviations: $A = \text{ch}\varphi - \cos\psi$, $B = \text{ch}\varphi\cos\psi - 1$, $C = \text{ch}\vartheta - \cos\psi$ and $D = \text{ch}\vartheta\cos\psi - 1$ are also employed. These results were used in this section to derive expressions for the elastic strain energy associated with the arrays.

3.1. *Screw dislocation array*

Consider an infinitely long array of screw dislocations. The stress components are periodic functions of y, with a period of p, so that along the planes $y = \pm np$, n being an integer, the shear stresses $\sigma_{zx}^{(1)}$ and $\sigma_{zx}^{(2)}$ are equal to zero. From eqns (B.2) and (B.4) of Appendix B it further follows that

$$\sigma_{zy}^{(1)}(x,0) = \frac{\mu_1 b_z}{2p}\left(\coth\frac{\vartheta}{2} - k_4 \coth\frac{\varphi}{2}\right) \tag{12}$$

$$\sigma_{zy}^{(2)}(x,0) = \frac{\mu_2 b_z}{2p}(1+k_4)\coth\frac{\vartheta}{2}. \tag{13}$$

The force on each dislocation in the array is $F_x = b_z\sigma_{zy}^{(1)}(h,0)$, which gives

$$F_x = -k_4\frac{\mu_1 b_z^2}{2p}\coth\varphi_0, \tag{14}$$

where $\varphi_0 = 2\pi h_0$. If dislocation spacing p is much greater than a distance h between the array and the interface ($\varphi_0 \to 0$), eqn (14) reduces to the force on an isolated screw dislocation near the interface. On the other hand, if h is much greater than p, the dislocation force approaches the constant value of $-k_4(\mu_1 b_z^2/2p)$.

Since

$$\frac{1}{h}\int_0^h \sigma_{zy}^{(1)}(x,y)\,\mathrm{d}x = \frac{\mu_1 b_z}{4\pi h}\ln\frac{1-\cos\psi}{\operatorname{ch}2\varphi_0 - \cos\psi}, \tag{15}$$

the average stress $\sigma_{zy}^{(1)}$ within the layer is

$$\sigma_{zy}^{0} = \frac{1}{hp}\int_{-p/2}^{p/2}\int_0^h \sigma_{zy}^{(1)}(x,y)\,\mathrm{d}x\,\mathrm{d}y = -(1+k_4)\frac{\mu_1 b_z}{2p}. \tag{16}$$

If a dislocation array is modeled by a continuous distribution of infinitesimal dislocations with density $1/p$ and the specific Burgers vector of magnitude b_z/p, the stresses are obtained by an appropriate integration. The result is the zero stress component σ_{zx} in both materials, and a discontinuous distribution of the stress component σ_{zy}, defined by

$$\sigma_{zy}^{(1)} = \begin{cases} -(1+k_4)\mu_1 b_z/2p, & x < h \\ (1-k_4)\mu_1 b_z/2p, & x > h \end{cases} \tag{17}$$

$$\sigma_{zy}^{(2)} = -(1+k_4)\frac{\mu_2 b_z}{2p}. \tag{18}$$

For $x < 0$ and $x > h$, the values of the shear stresses (17) and (18) are the far-field stresses of the array with a discrete dislocation distribution. Also, the value of the shear stress (17) for $x < h$ is the average stress σ_{zy}^0 in the layer for an array with discrete dislocation distribution, given by eqn (16).

The strain energy per unit dislocation length within a horizontal strip of large length $2R$ and width p, associated with introduction of the dislocation array in an initial configuration under uniform stress σ_{zy}^0, can be written as

$$E = E_* + b_z\sigma_{zy}^0(R-h) + E_0, \tag{19}$$

where E_0 is the strain energy in the initial configuration, and

$$E_{*} = \frac{1}{2} b_z \int_{h+\rho}^{R} [\sigma_{zy}^{(1)}(x,0) - \sigma_{zy}^{0}]\, dx. \tag{20}$$

There is no coefficient of one-half in front of the second term on the right-hand side of eqn (19), since the stress σ_{zy}^0 is considered to be already applied before the subsequent introduction of slip discontinuity b_z along the cut $x \geqslant h$. Substitution of eqn (12) into eqn (20), followed by integration yields

$$E_{*} = \frac{\mu_1 b_z^2}{4\pi}\left[\ln\frac{\operatorname{sh}\varphi_0}{\operatorname{sh}\rho_0} - (1+k_4)\varphi_0 - (1-k_4)\ln(2\operatorname{sh}\varphi_0) + 2R_0\right], \tag{21}$$

where $R_0 = \pi R/p$, and $\rho_0 = \pi\rho/p$. Thus, the strain energy is

$$E = \frac{\mu_1 b_z^2}{4\pi}\left[\ln\frac{\operatorname{sh}\varphi_0}{\operatorname{sh}\rho_0} - (1-k_4)\ln(2\operatorname{sh}\varphi_0) - 2k_4 R_0\right] + E_0. \tag{22}$$

If the array is near the free surface of a semi-infinite body, it follows that $\sigma_{zy}^0 = -\mu_1 b_z/p$, $E_0 = R_0\mu_1 b_z^2/2\pi$, and the strain energy becomes

$$E = \frac{\mu_1 b_z^2}{4\pi}\ln\frac{\operatorname{sh}\varphi_0}{\operatorname{sh}\rho_0}. \tag{23}$$

For a sufficiently small core radius, $\operatorname{sh}\rho_0$ in eqn (23) can be replaced with ρ_0.

3.2. *Edge dislocation array with the Burgers vector normal to the interface*

Consider an infinitely long dislocation array at a distance h from the interface of two joined materials (Fig. 2). The array consists of identical, uniformly spaced edge dislocations with their Burgers vectors normal to the interface. Such an array is commonly referred to

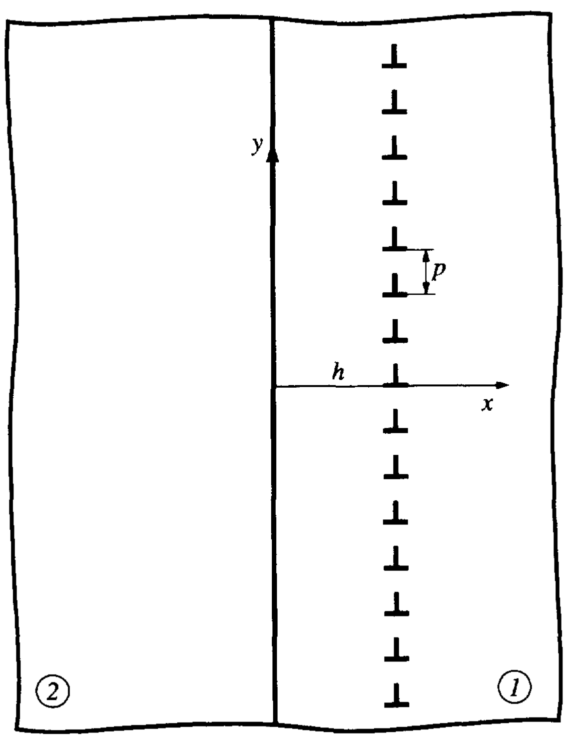

Fig. 2. A dislocation wall of spacing p at a distance h from the bimaterial interface. The Burgers vector of each dislocation is normal to the interface.

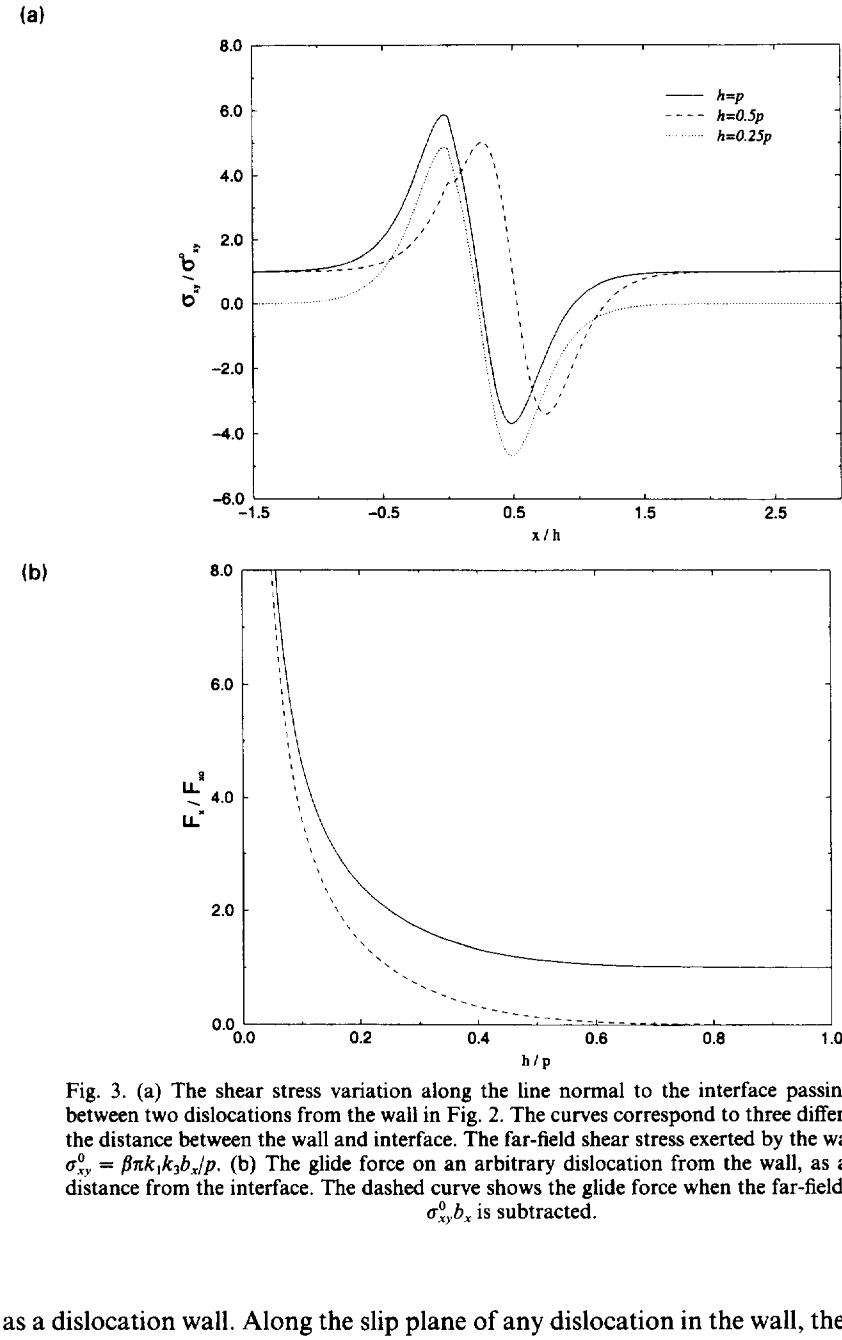

Fig. 3. (a) The shear stress variation along the line normal to the interface passing exactly in-between two dislocations from the wall in Fig. 2. The curves correspond to three different values of the distance between the wall and interface. The far-field shear stress exerted by the wall is equal to $\sigma_{xy}^0 = \beta\pi k_1 k_3 b_x/p$. (b) The glide force on an arbitrary dislocation from the wall, as a function of distance from the interface. The dashed curve shows the glide force when the far-field value $F_{xo} = \sigma_{xy}^0 b_x$ is subtracted.

as a dislocation wall. Along the slip plane of any dislocation in the wall, the normal stresses σ_x and σ_y are equal to zero. From eqns (B.7) and (B.10), the corresponding shear stress is

$$\sigma_{xy}^{(1)}(x,0) = \frac{\pi k_1 b_x}{p}\left\{\frac{\vartheta}{2\,\mathrm{sh}^2(\vartheta/2)} + \frac{k_2}{2\,\mathrm{sh}^2(\varphi/2)}[\vartheta + 2c(\varphi)] + \beta k_3 \coth\frac{\varphi}{2}\right\} \tag{24}$$

$$\sigma_{xy}^{(2)}(x,0) = \frac{\pi k_1 k_3 b_x}{p}\,\frac{\vartheta + \beta(\varphi - \mathrm{sh}\,\vartheta)}{2\,\mathrm{sh}^2(\vartheta/2)}, \tag{25}$$

where $c(\varphi) = \varphi_0(\varphi - \varphi_0)\coth(\varphi/2)$. Figure 3(a) shows the variation of this shear stress in the case of an aluminum/copper bimaterial, for which $\mu_1 = 26$ GPa, $\nu_1 = 0.33$, $\mu_2 = 45$ GPa, $\nu_2 = 0.35$. Substitution of these values into eqn (2) yields the following values of the Dundurs parameters: $\alpha = 0.28$ and $\beta = 0.08$, so from eqn (1), $k_2 = 0.185$ and $k_3 = 1.288$. The plots correspond to the walls at distance $h = 0.25p$, $0.5p$ and p from the interface. The non-vanishing far-field shear stress $\sigma_{xy}^0 = \beta\pi k_1 k_3 b_x/p$ is quickly approached away from the wall. The significance of this far-field stress in connection with a grain boundary modeling and Frank's formula has been discussed by Chou and Lin (1975), and Hirth *et al.* (1979). The latter authors suggested to subtract the far-field shear stress in order to simulate the grain boundary in an unloaded bicrystal of finite size. With the increase of h, the non-vanishing shear stress pattern in a narrow region around the wall translates with the wall, preserving its shape and magnitude. Figure 3(b) shows the glide force on an arbitrary dislocation from the wall, obtained according to eqn (27) below, as a function of a distance h from the interface. When the far-field value is subtracted (dashed curve), the glide force quickly decreases to essentially a zero value, at a distance h from the interface of the order of dislocation spacing p. Beyond this distance, the wall is in an approximate equilibrium configuration (Hirth *et al.*, 1979), without further observable tendency to move away from the interface. See also Gutkin *et al.* (1989), and Gutkin and Romanov (1994), who studied the location of this stand-off position of misfit dislocations.

If a dislocation wall with uniformly spaced edge dislocations of spacing p is modeled by a continuous distribution of infinitesimal dislocations with density $1/p$, the stresses are obtained by an appropriate integration. The result is a uniform stress distribution in both materials

$$\sigma_x = \sigma_y = 0, \quad \sigma_{xy} = \sigma_{xy}^0 = \beta\frac{\pi k_1 k_3 b_x}{p}. \tag{26}$$

This also represents the far field stresses (at $x \to \pm\infty$) of the previously considered discrete wall.

The glide force on each dislocation from the wall is $F_x = b_x\sigma_{xy}^{(1)}(h,0)$. The divergent part of the shear stress $\sigma_{xy}^{(1)}(h,0)$, due to the ϑ/C term at $x = h$, has been excluded. This gives

$$F_x = \frac{\pi k_1 b_x^2}{p}\coth\varphi_0\left(\beta k_3 + k_2\frac{\varphi_0^2}{\mathrm{sh}^2\,\varphi_0}\right). \tag{27}$$

If dislocation spacing p is much greater than a distance h between the wall and the interface, eqn (27) reduces to the glide force of a single dislocation near the interface. On the other hand, if h is much greater than p, the glide force on a dislocation in the wall approaches the constant value of $\beta\pi k_1 k_3 b_x^2/p$. This is equal to zero only if the two materials are identical, or incompressible (since then $\beta = 0$), or if the wall is located in a semi-infinite body with the traction free boundary $x = 0$ (since then $\alpha = -1$ and $k_3 = 0$).

The strain energy per unit dislocation length within a horizontal strip of large length $2R$ and width p, excluding the dislocation core, associated with introduction of the dislocation wall in an initial configuration under uniform stress σ_{xy}^0, can be written as

$$E = E_* + b_x\sigma_{xy}^0(R-h) - E_\rho + E_0. \tag{28}$$

Here, E_ρ is the energy associated with tractions applied on a core surface of radius ρ, E_0 is the strain energy in the initial configuration, and

$$E_* = \frac{1}{2}b_x\int_{h+\rho}^{R}[\sigma_{xy}^{(1)}(x,0) - \sigma_{xy}^0]\,\mathrm{d}x. \tag{29}$$

There is no coefficient of one half in front of the second term on the right-hand side of eqn (28), since the stress σ_{xy}^0 was considered already applied before the subsequent introduction of slip discontinuity b_x along the cut $x \geqslant h$. Recall that the stress σ_{xy}^0 is the far field shear stress and also the average stress σ_{xy} in the layer between the array and the interface. Substitution of eqn (24) into eqn (29) and integration yields

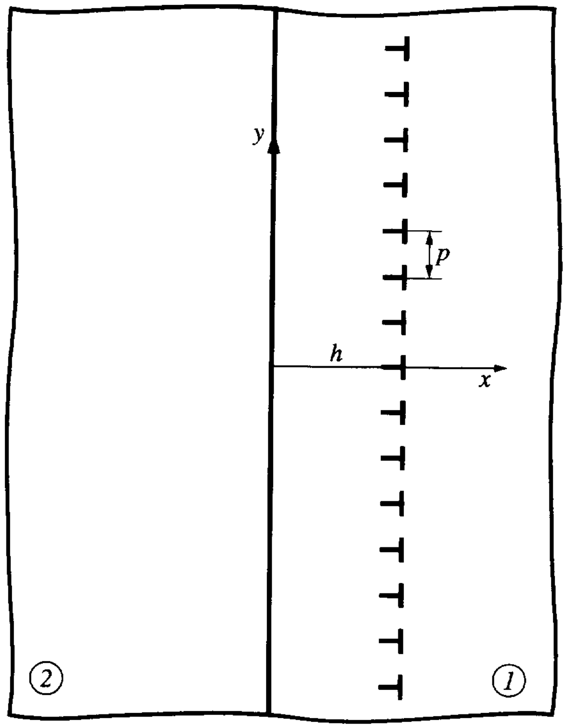

Fig. 4. Dislocation array of spacing p at a distance h from the bimaterial interface. The Burgers vector of each dislocation is parallel to the interface.

$$E_* = \frac{1}{2}k_1 b_x^2\left\{\ln\frac{\operatorname{sh}\varphi_0}{\operatorname{sh}\rho_0} + \rho_0\coth\rho_0 + k_2\left(\varphi_0\coth\varphi_0 + \frac{\varphi_0^2}{2\operatorname{sh}^2\varphi_0}\right) + k_3[\beta\varphi_0 - \ln(2\operatorname{sh}\varphi_0)]\right\}. \tag{30}$$

Again, for a sufficiently small core radius (relative to h and p), E_p can be calculated by replacing the dislocation core with a cylindrical hole, whose surface is subjected to tractions of an isolated dislocation in an infinite homogeneous body, along with the corresponding displacements. Hence, E_p in eqn (28) is independent of h, and equal to $k_1 b_x^2(1-2\nu_1)/8(1-\nu_1)$.

If the wall is near the free surface in a semi-infinite body ($k_2 = -1, k_3 = 0$), the far-field shear stress is equal to zero, and $E_0 = 0$. Hence, neglecting the energy of the ledges left on the free surface, the energy is $E = E_* - E_p$, with the corresponding simplifications in the expression (30) due to $k_2 = -1$ and $k_3 = 0$. The glide force on a dislocation is in this case $F_x = -(\pi k_1 b_x^2/p)\varphi_0^2 \operatorname{ch}\varphi_0/\operatorname{sh}^3\varphi_0$.

3.3. *Dislocation array with the Burgers vector parallel to the interface*

The stress components for a dislocation array with the dislocation Burgers vector parallel to the interface (Fig. 4) are given by eqns (B.14)–(B.19) of Appendix B. Along the line $y = 0$, or any parallel line passing through the dislocation in the array, the shear stress σ_{xy} is equal to zero, while the normal stress σ_y becomes

$$\sigma_y^{(1)}(x,0) = \frac{\pi k_1 b_y}{p}\left\{\frac{2\operatorname{sh}\vartheta - \vartheta}{2\operatorname{sh}^2(\vartheta/2)} + \frac{k_2}{2\operatorname{sh}^2(\varphi/2)}[2\operatorname{sh}\varphi - \varphi - 2\varphi_0 + 2c(\varphi)] + \beta k_3\coth\frac{\varphi}{2}\right\} \tag{31}$$

$$\sigma_y^{(2)}(x,0) = \frac{\pi k_1 k_3 b_y}{p}\frac{2\operatorname{sh}\vartheta - \vartheta + \beta(\operatorname{sh}\vartheta - \varphi)}{2\operatorname{sh}^2(\varphi/2)}. \tag{32}$$

(a)

(b)

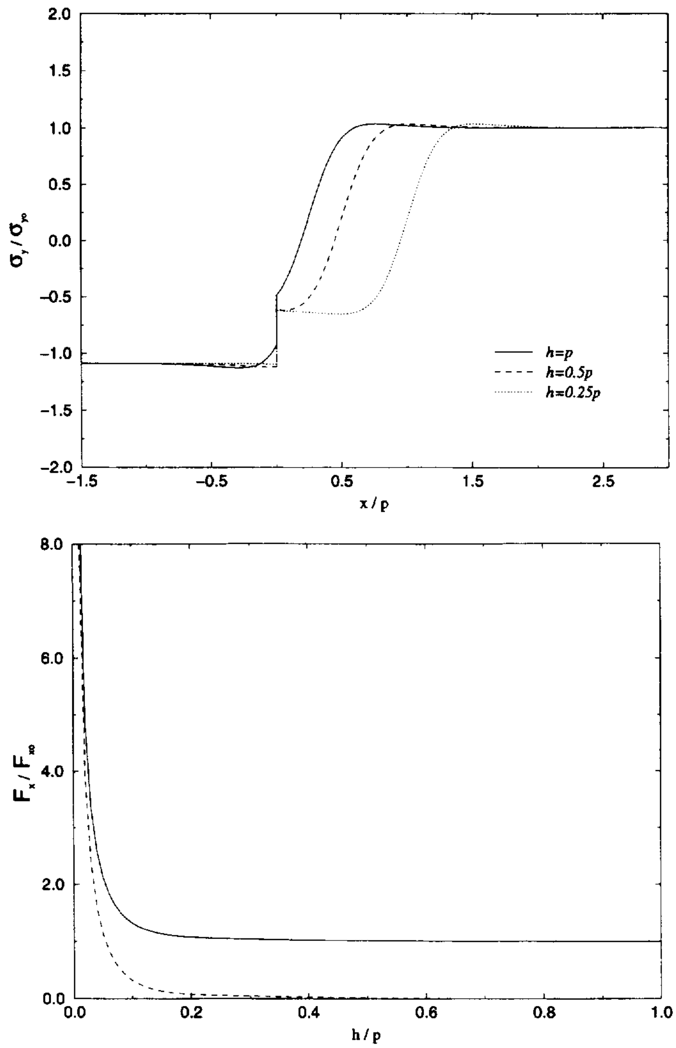

Fig. 5. (a) The normal stress variation along the line normal to the interface passing exactly in between two dislocations from the array in Fig. 4. The far-field value of σ_y at $x \to \infty$ is $\sigma_{y0} = \pi k_1 k_3 b_y (2-\beta)/p$. (b) The climb force on an arbitrary dislocation from the array, as a function of a distance from the interface. The dashed curve shows the climb force when the far-field value $F_{xo} = (\pi k_1 b_y^2/p)[k_3(2-\beta)-2]$ is subtracted.

Figure 5(a) shows the variation of the normal stress σ_y along the line $y = 0$ for the previously considered aluminum/copper bimaterial. The variation is shown for the arrays at distance $h = 0.25p$, $0.5p$ and p from the interface. For h greater than p, the stress is approximately constant in the region between the array and interface. The stress quickly sets in to a constant, but different values in the rest of material (1) and material (2). Figure 5(b) shows the change of the climb force as a function of a distance between the array and the interface, determined by eqn (35) below.

If a dislocation array is modeled by a continuous distribution of infinitesimal dislocations, the result is a uniform distribution of stress $\sigma_x = \sigma_x^0 = \beta\pi k_1 k_3 b_y/p$ and $\sigma_{xy} = 0$ throughout both materials, and a discontinuous distribution of the stress component σ_y defined by

$$\sigma_y^{(1)} = \begin{cases} k_3(2-\beta)\pi k_1 b_y/p, & x > h \\ [k_3(2-\beta)-4]\pi k_1 b_y/p, & x < h \end{cases} \tag{33}$$

$$\sigma_y^{(2)} = -k_3(2+\beta)\pi k_1 b_y/p. \tag{34}$$

The stress between the array and interface is $\sigma_y^0 = [k_3(2-\beta)-4]\pi k_1 b_y/p$. If the array is parallel to the free surface of a semi-infinite homogeneous body ($k_3 = 0$), there is a constant stress σ_y of magnitude $4\pi k_1 b_y/p$ between the array and the free surface, and a zero stress behind the array. Herring (1951) suggested that a dislocation array just beneath the free surface will spontaneously form if the lowering of the surface energy caused by the array is greater than the strain energy of the array itself. For most materials this condition is not satisfied, although for some materials it could be, particularly for those with a compressive rather than tensile surface stress. Hartley (1969) has also discussed the nature of the stress field produced by the array in connection with a tendency for the segregation of impurities between the array and the free surface. Freund *et al.* (1993) studied the equilibrium surface roughness and mass rearrangement induced by a non-uniform stress field due to dislocations just below the surface.

The climb force on a dislocation from the array is found to be

$$F_x = \frac{\pi k_1 b_y^2}{p}\coth\varphi_0\left[\beta k_3 + 2k_2\left(1+\frac{\varphi_0^2}{2\,\mathrm{sh}^2\,\varphi_0}-\frac{2\varphi_0}{\mathrm{sh}\,2\varphi_0}\right)\right]. \tag{35}$$

If the dislocation spacing p is much greater than the distance h between the array and the interface, eqn (35) gives the climb force for a single dislocation near the interface. On the other hand, if h is much greater than p, the climb force approaches the constant value

$$F_x = \frac{\pi k_1 b_y^2}{p}[k_3(2-\beta)-2]. \tag{36}$$

This force is equal to zero only if two materials are identical, since then $\beta = 0$, and $k_3 = 1$. Expression for the climb force (36) can also be obtained from eqn (33) by using the mean value of the stress $\sigma_y^{(1)}$ at $x = h \pm 0$.

The strain energy associated with introduction of the dislocation array in an initial configuration under uniform normal stress σ_x^0, and σ_y^0, can be written as

$$E = E_* + b_y\sigma_y^0(R-h) - E_\rho + E_0, \tag{37}$$

where

$$E_* = \frac{1}{2}b_y\int_{h+\rho}^{R}[\sigma_y^{(1)}(x,0)-\sigma_y^0]\,\mathrm{d}x. \tag{38}$$

The stress σ_y^0 appears in the above energy expressions due to the fact that, when a dislocation array moves from a distance h to a distance $R \gg h$ from the interface, the stress $\sigma_y^{(1)}$ left behind the array is σ_y^0. Substitution of eqn (31) into (38) and integration gives

$$E_* = \frac{1}{2}k_1 b_y^2\left\{\ln\frac{\mathrm{sh}\,\varphi_0}{\mathrm{sh}\,\rho_0} - \rho_0\coth\rho_0 - k_2\left(\varphi_0\coth\varphi_0 - \frac{\varphi_0^2}{2\,\mathrm{sh}^2\,\varphi_0}\right)\right.$$
$$\left. + k_3[(2-\beta)\varphi_0 - \ln(2\,\mathrm{sh}\,\varphi_0)] + 4(R_0-\varphi_0)\right\}. \tag{39}$$

If the array is near the free surface of a semi-infinite body ($k_2 = -1, k_3 = 0$), it follows that $\sigma_y^0 = -4\pi k_1 b_y/p$, and $E_0 = 2k_1 b_y^2 R_0$. Hence, the total strain energy per unit dislocation length within a strip of width p is

$$E = \frac{1}{2}k_1 b_y^2\left(\ln\frac{\mathrm{sh}\,\varphi_0}{\mathrm{sh}\,\rho_0} - \rho_0\coth\rho_0 + \varphi_0\coth\varphi_0 - \frac{\varphi_0^2}{2\,\mathrm{sh}^2\,\varphi_0}\right) - E_\rho. \tag{40}$$

4. THE ENERGY OF A GENERAL STRAIGHT DISLOCATION ARRAY

Results for a general dislocation array, whose dislocations have the Burgers vectors with the edge and screw components, are now derived. The strain energy associated with the introduction of a dislocation array in an initial configuration under uniform stress distribution σ_y^0, σ_{xy}^0 and σ_{zy}^0, is

$$E = E_* + (\sigma_{xy}^0 b_x + \sigma_y^0 b_y + \sigma_{zy}^0 b_z)(R-h) - E_\rho + E_0, \tag{41}$$

where

$$E_* = \frac{1}{2}\int_{h+\rho}^{R} \{b_x[\sigma_{xy}^{(1)}(x,0) - \sigma_{xy}^0] + b_y[\sigma_y^{(1)}(x,0) - \sigma_y^0] + b_z[\sigma_{zy}^{(1)}(x,0) - \sigma_{zy}^0]\}\,\mathrm{d}x. \tag{42}$$

Recall that σ_{xy}^0, σ_y^0 and σ_{zy}^0 represent the average stresses in the layer between the dislocation array and the interface, and are given by $\sigma_y^0 = \pi k_1 b_y[k_3(2-\beta)-4]/p$, $\sigma_{xy}^0 = \beta\pi k_1 k_3 b_x/p$, and $\sigma_{zy}^0 = -\pi k_1 b_z(1-\nu_1)(1+k_4)/p$. Combining results from the previous subsections, it now easily follows that

$$E = \frac{k_1}{2}\left\{(b_x^2+b_y^2)\left[\ln\frac{\operatorname{sh}\varphi_0}{\operatorname{sh}\rho_0} + k_2\frac{\varphi_0^2}{2\operatorname{sh}^2\varphi_0} - k_3\ln(2\operatorname{sh}\varphi_0)\right]\right.$$
$$+ (b_x^2-b_y^2)(\rho_0\coth\rho_0 + k_2\varphi_0\coth\varphi_0 + 2\beta k_3 R_0) - 4b_y^2(1-k_3)R_0$$
$$\left. + (1-\nu_1)b_z^2\left[\ln\frac{\operatorname{sh}\varphi_0}{\operatorname{sh}\rho_0} - (1-k_4)\ln(2\operatorname{sh}\varphi_0) - 2k_4R_0\right]\right\} - E_\rho + E_0. \tag{43}$$

The force on a dislocation is obtained from eqn (43) as a negative gradient with respect to h, which gives

$$F_x = -\frac{\pi k_1}{p}\coth\varphi_0\left\{(b_x^2+b_y^2)\left[1-k_3+k_2\frac{2\varphi_0}{\operatorname{sh}2\varphi_0}(1-\varphi_0\coth\varphi_0)\right]\right.$$
$$\left. + (b_x^2-b_y^2)k_2\left(1-\frac{2\varphi_0}{\operatorname{sh}2\varphi_0}\right) + (1-\nu_1)b_z^2k_4\right\}. \tag{44}$$

If the array is near the free surface of a semi-infinite body, the strain energy of the initial configuration is $E_0 = k_1[2b_y^2 + (1-\nu_1)b_z^2]R_0$. With the core contribution E_ρ given by eqn (10), the energy expression (43) simplifies to

$$E = \frac{k_1}{2}\left\{(b_x^2+b_y^2)\left[\ln\frac{\operatorname{sh}\varphi_0}{\operatorname{sh}\rho_0} - \frac{\varphi_0^2}{2\operatorname{sh}^2\varphi_0} + \frac{1}{4(1-\nu_1)}\right]\right.$$
$$\left. + (b_x^2-b_y^2)\left(\frac{1}{2}-\varphi_0\coth\varphi_0\right) + (1-\nu_1)b_z^2\ln\frac{\operatorname{sh}\varphi_0}{\operatorname{sh}\rho_0}\right\}. \tag{45}$$

For a sufficiently small core radius $\operatorname{sh}\rho_0$ can be replaced by ρ_0. Equation (45) is in agreement with eqn (17) of Willis *et al.* (1991). For comparison, their energy E_d is related to our E by $E = E_d - E_\rho - h(\sigma_y^0 b_y + \sigma_{zy}^0 b_z)/2$. If $h \ll p$, eqn (45) reduces to eqn (11) for an isolated dislocation near the free surface. If $h \gg p$, eqn (45) gives $E = [2b_y^2 + (1-\nu_1)b_z^2]\pi k_1 h/p$, which is proportional to h. This is so because for $h \gg p$ the stress field in the layer becomes essentially constant ($\sigma_y = \sigma_y^0 = -4\pi k_1 b_y/p$, and $\sigma_{zy} = \sigma_{zy}^0 = -\mu_1 b_z/p$), as if the array consists of continuously distributed infinitesimal dislocations.

5. CONCLUDING REMARKS

The main results of this paper are the energy expressions (43)–(45), and the formulas for the complete stress distribution in a bimaterial due to dislocation arrays parallel to bimaterial interface. Expression (43) represents the elastic strain energy per unit dislocation length within a considered segment of an infinite bimaterial body, produced by periodic dislocation array parallel to a bimaterial interface. Expression (44) gives the corresponding force exerted on each dislocation in the array. Expression (45) is a special case of eqn (43), and gives the elastic strain energy produced by dislocation array near the free surface of a semi-infinite homogeneous body. This expression is important in the analysis of strain relaxation processes in thin films bonded to their substrates (Lubarda, 1996). Expressions for the complete stress distribution are listed in Appendix B.

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APPENDIX A

A.1. *Screw dislocation*

The only non-vanishing displacement component for a screw dislocation with the Burgers vector b_z, at a distance h from a bimaterial interface, is

$$u_z^{(1)} = \frac{b_z}{2\pi}(\theta_1 - k_4\theta_2) \tag{A1}$$

$$u_z^{(2)} = \frac{b_z}{2\pi}[(1+k_4)\theta_1 - \pi k_4]. \tag{A2}$$

The constant k_4 is defined in eqn (1), and the angles θ_1 and θ_2 are shown in Fig. A1. The associated stresses are

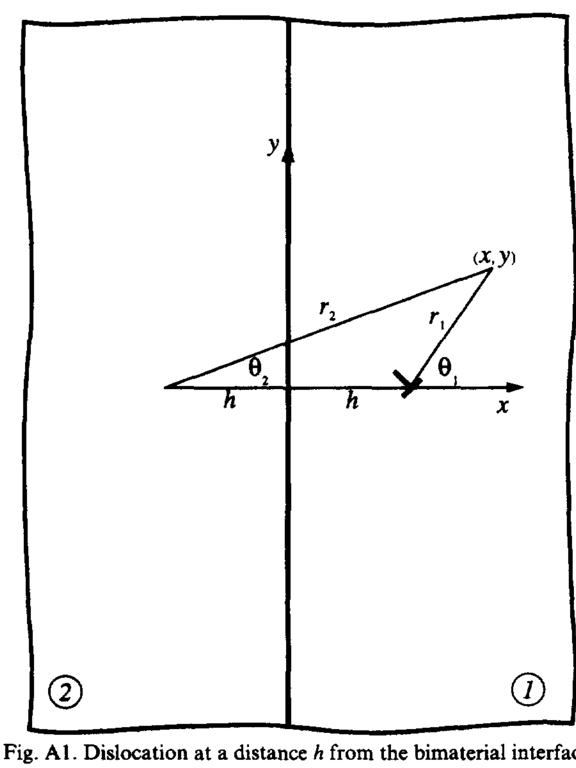

Fig. A1. Dislocation at a distance h from the bimaterial interface.

$$\sigma_{zx}^{(1)} = -\frac{\mu_1 b_z}{2\pi}\left(\frac{y}{r_1^2} - k_4\frac{y}{r_2^2}\right) \tag{A3}$$

$$\sigma_{zy}^{(1)} = \frac{\mu_1 b_z}{2\pi}\left(\frac{x-h}{r_1^2} - k_4\frac{x+h}{r_2^2}\right), \tag{A4}$$

and

$$\sigma_{zx}^{(2)} = -\frac{\mu_2 b_z}{2\pi}(1+k_4)\frac{y}{r_1^2} \tag{A5}$$

$$\sigma_{zy}^{(2)} = \frac{\mu_2 b_z}{2\pi}(1+k_4)\frac{x-h}{r_1^2}. \tag{A6}$$

The polar coordinates shown in Fig. A1 are employed, so that in terms of the Cartesian (x,y) coordinates $r_1^2 = (x-h)^2+y^2$, $r_2^2 = (x+h)^2+y^2$, $\tan\theta_1 = y/(x-h)$, and $\tan\theta_2 = y/(x+h)$.

A.2. *Edge dislocation with the Burgers vector* b_x

The Airy stress function for the stress field due to edge dislocation with the Burgers vector b_x is (Dundurs, 1969)

$$\Phi^{(1)} = -k_1 b_x\left[r_1 \ln r_1 \sin\theta_1 + (k_3-1)r_2 \ln r_2 \sin\theta_2 - k_2 h\left(\sin 2\theta_2 - 2h\frac{\sin\theta_2}{r_2}\right) + \beta k_3 r_2\theta_2\cos\theta_2\right] \tag{A7}$$

$$\Phi^{(2)} = -k_1 k_3 b_x[r_1 \ln r_1 \sin\theta_1 - \beta(r_1\theta_1\cos\theta_1 + 2h\theta_1)]. \tag{A8}$$

The corresponding stresses are

$$\sigma_x^{(1)} = -k_1 b_x\left\{\frac{y[3(x-h)^2+y^2]}{r_1^4} + k_2\frac{y[3(x+h)^2+y^2]}{r_2^4} + 4k_2 hxy\frac{3(x+h)^2-y^2}{r_2^6} + \beta k_3\frac{y}{r_2^2}\right\} \tag{A9}$$

$$\sigma_y^{(1)} = k_1 b_x\left\{\frac{y[(x-h)^2-y^2]}{r_1^4} + k_2\frac{y[(x+h)^2-y^2]}{r_2^4} - 4k_2 hy\frac{2(x+h)^3-3x(x+h)^2+2(x+h)y^2+xy^2}{r_2^6} + \beta k_3\frac{y}{r_2^2}\right\} \tag{A10}$$

$$\sigma_{xy}^{(1)} = k_1 b_x\left\{\frac{(x-h)[(x-h)^2-y^2]}{r_1^4} + k_2\frac{(x+h)[(x+h)^2-y^2]}{r_2^4} - 2k_2 h\frac{(x+h)^4-2x(x+h)^3+6x(x+h)y^2-y^4}{r_2^6} + \beta k_3\frac{x+h}{r_2^2}\right\}, \tag{A11}$$

and

$$\sigma_x^{(2)} = -k_1 k_3 b_x\left\{\frac{y[3(x-h)^2+y^2]}{r_1^4} + 2\beta y\frac{x^2-h^2}{r_1^4}\right\} \tag{A12}$$

$$\sigma_y^{(2)} = k_1 k_3 b_x\left\{\frac{y[(x-h)^2-y^2]}{r_1^4} + 2\beta y\frac{2h(x-h)-y^2}{r_1^4}\right\} \tag{A13}$$

$$\sigma_{xy}^{(2)} = k_1 k_3 b_x\left\{\frac{(x-h)[(x-h)^2-y^2]}{r_1^4} + 2\beta\frac{h(x-h)^2-xy^2}{r_1^4}\right\}. \tag{A14}$$

A.3. *Edge dislocation with the Burgers vector* b_y

For an edge dislocation with the Burgers vector b_y, the Airy stress function is

$$\Phi^{(1)} = k_1 b_y\left[r_1 \ln r_1 \cos\theta_1 + (k_3-1)r_2 \ln r_2 \cos\theta_2 - k_2 h\left(2\ln r_2 - \cos 2\theta_2 + 2h\frac{\cos\theta_2}{r_2}\right) - \beta k_3 r_2\theta_2 \sin\theta_2\right] \tag{A15}$$

$$\Phi^{(2)} = k_1 k_3 b_y[r_1 \ln r_1 \cos\theta_1 + \beta(2h\ln r_1 + r_1\theta_1\sin\theta_1)]. \tag{A16}$$

The stress components are

$$\sigma_x^{(1)} = k_1 b_y \left\{ \frac{(x-h)[(x-h)^2-y^2]}{r_1^4} + k_2 \frac{(x+h)[(x+h)^2-y^2]}{r_2^4} - 2k_2 h \frac{(x+h)^4+2x(x+h)^3-6x(x+h)y^2-y^4}{r_2^6} - \beta k_3 \frac{x+h}{r_2^2} \right\} \quad \text{(A17)}$$

$$\sigma_y^{(1)} = k_1 b_y \left\{ \frac{(x-h)[(x-h)^2+3y^2]}{r_1^4} + k_2 \frac{(x+h)[(x+h)^2+3y^2]}{r_2^4} - 2k_2 h \frac{(x+h)^4-2x(x+h)^3+6x(x+h)y^2-y^4}{r_2^6} + \beta k_3 \frac{x+h}{r_2^2} \right\} \quad \text{(A18)}$$

$$\sigma_{xy}^{(1)} = k_1 b_y \left\{ \frac{y[(x-h)^2-y^2]}{r_1^4} + k_2 \frac{y[(x+h)^2-y^2]}{r_2^4} - 4k_2 hxy \frac{3(x+h)^2-y^2}{r_2^6} - \beta k_3 \frac{y}{r_2^2} \right\}, \quad \text{(A19)}$$

and

$$\sigma_x^{(2)} = k_1 k_3 b_y \left\{ \frac{(x-h)[(x-h)^2-y^2]}{r_1^4} + 2\beta \frac{x(x-h)^2-hy^2}{r_1^4} \right\} \quad \text{(A20)}$$

$$\sigma_y^{(2)} = k_1 k_3 b_y \left\{ \frac{(x-h)[(x-h)^2+3y^2]}{r_1^4} - 2\beta \frac{h(x-h)^2-xy^2}{r_1^4} \right\} \quad \text{(A21)}$$

$$\sigma_{xy}^{(2)} = k_1 k_3 b_y \left\{ \frac{y[(x-h)^2-y^2]}{r_1^4} + 2\beta y \frac{x^2-h^2}{r_1^4} \right\}. \quad \text{(A22)}$$

APPENDIX B

This appendix gives expressions for the stress components in a bimaterial due to three types of dislocation arrays parallel to bimaterial interface. The expressions are obtained by appropriate summations of the stress fields due to individual dislocations, listed in Appendix A. The following non-dimensional variables are employed: $\xi = x/p$, $\eta = y/p$, $h_0 = h/p$ and $\vartheta = 2\pi(\xi - h_0)$, $\varphi = 2\pi(\xi + h_0)$, $\psi = 2\pi\eta$. The abbreviations: $A = \operatorname{ch}\varphi - \cos\psi$, $B = \operatorname{ch}\varphi\cos\psi - 1$, $C = \operatorname{ch}\vartheta - \cos\psi$ and $D = \operatorname{ch}\vartheta\cos\psi - 1$ are also used.

B.1. *Screw dislocation array*

$$\sigma_{zx}^{(1)} = -\frac{\mu_1 b_z}{2p} \sin\psi \left(\frac{1}{C} - k_4 \frac{1}{A} \right) \quad \text{(B1)}$$

$$\sigma_{zy}^{(1)} = \frac{\mu_1 b_z}{2p} \left(\frac{\operatorname{sh}\vartheta}{C} - k_4 \frac{\operatorname{sh}\varphi}{A} \right), \quad \text{(B2)}$$

and

$$\sigma_{zx}^{(2)} = -\frac{\mu_2 b_z}{2p} (1+k_4) \frac{\sin\psi}{C} \quad \text{(B3)}$$

$$\sigma_{zy}^{(2)} = \frac{\mu_2 b_z}{2p} (1+k_4) \frac{\operatorname{sh}\vartheta}{C}. \quad \text{(B4)}$$

B.2. *Edge dislocation array with the Burgers vector* $\mathbf{b}_x$

$$\sigma_x^{(1)} = -\frac{\pi k_1 b_x \sin\psi}{A^2 p} (X_1 + k_2 X_2 + \beta k_3 X_3) \quad \text{(B5)}$$

$$\sigma_y^{(1)} = \frac{\pi k_1 b_x \sin\psi}{A^2 p} (Y_1 + k_2 Y_2 + \beta k_3 Y_3) \quad \text{(B6)}$$

$$\sigma_{xy}^{(1)} = \frac{\pi k_1 b_x}{A^2 p} (T_1 + k_2 T_2 + \beta k_3 T_3), \quad \text{(B7)}$$

and

$$\sigma_x^{(2)} = -\frac{\pi k_1 k_3 b_x \sin\psi}{C^2 p}[(\vartheta\,\mathrm{sh}\,\vartheta + C) + \beta\varphi\,\mathrm{sh}\,\vartheta] \quad \text{(B8)}$$

$$\sigma_y^{(2)} = \frac{\pi k_1 k_3 b_x \sin\psi}{C^2 p}[(\vartheta\,\mathrm{sh}\,\vartheta - C) + \beta(4\pi\xi\,\mathrm{sh}\,\vartheta - \vartheta\,\mathrm{sh}\,\vartheta - 2C)] \quad \text{(B9)}$$

$$\sigma_{xy}^{(2)} = \frac{\pi k_1 k_3 b_x}{C^2 p}[D\vartheta - \beta(C\,\mathrm{sh}\,\vartheta - D\varphi)]. \quad \text{(B10)}$$

In eqns (B5)–(B10), the following abbreviations were used: $X_1 = (A/C)^2(\vartheta\,\mathrm{sh}\,\vartheta + C)$, $Y_1 = (A/C)^2(\vartheta\,\mathrm{sh}\,\vartheta - C)$, $T_1 = (A/C)^2 D\vartheta$,

$$X_2 = \varphi\,\mathrm{sh}\,\varphi + A + \frac{8h_0\pi^2\xi}{A}(\mathrm{sh}^2\,\varphi + B) \quad \text{(B11)}$$

$$Y_2 = (\vartheta - 4h_0\pi)\,\mathrm{sh}\,\varphi - A + \frac{8h_0\pi^2\xi}{A}(\mathrm{sh}^2\,\varphi + B) \quad \text{(B12)}$$

$$T_2 = B\vartheta + \frac{8h_0\pi^2\xi}{A}\,\mathrm{sh}\,\varphi(B - \sin^2\psi), \quad \text{(B13)}$$

and $X_3 = Y_3 = A$, $T_3 = A\,\mathrm{sh}\,\varphi$.

B.3. *Edge dislocation array with the Burgers vector* $\mathbf{b}_y$

$$\sigma_x^{(1)} = \frac{\pi k_1 b_y}{A^2 p}(X_1 + k_2 X_2 + \beta k_3 X_3) \quad \text{(B14)}$$

$$\sigma_y^{(1)} = \frac{\pi k_1 b_y}{A^2 p}(Y_1 + k_2 Y_2 + \beta k_3 Y_3) \quad \text{(B15)}$$

$$\sigma_{xy}^{(1)} = \frac{\pi k_1 b_y \sin\psi}{A^2 p}(T_1 + k_2 T_2 + \beta k_3 T_3), \quad \text{(B16)}$$

and

$$\sigma_x^{(2)} = \frac{\pi k_1 k_3 b_y}{C^2 p}[D\vartheta + \beta(C\,\mathrm{sh}\,\vartheta + D\varphi)] \quad \text{(B17)}$$

$$\sigma_y^{(2)} = \frac{\pi k_1 k_3 b_y}{C^2 p}[(2C\,\mathrm{sh}\,\vartheta - D\vartheta) + \beta(C\,\mathrm{sh}\,\vartheta - D\varphi)] \quad \text{(B18)}$$

$$\sigma_{xy}^{(2)} = \frac{\pi k_1 k_3 b_y \sin\psi}{C^2 p}[(\vartheta\,\mathrm{sh}\,\vartheta - C) + \beta\varphi\,\mathrm{sh}\,\vartheta]. \quad \text{(B19)}$$

In expressions (B14)–(B19), the following abbreviations were used: $X_1 = (A/C)^2 D\vartheta$, $Y_1 = (A/C)^2(2C\,\mathrm{sh}\,\vartheta - D\vartheta)$, $T_1 = (A/C)^2(\vartheta\,\mathrm{sh}\,\vartheta - C)$,

$$X_2 = B\vartheta - \frac{8h_0\pi^2\xi}{A}\,\mathrm{sh}\,\varphi(B - \sin^2\psi) \quad \text{(B20)}$$

$$Y_2 = 2A\,\mathrm{sh}\,\varphi - (\varphi + 4h_0\pi)B + \frac{8h_0\pi^2\xi}{A}\,\mathrm{sh}\,\varphi(B - \sin^2\psi) \quad \text{(B21)}$$

$$T_2 = \varphi\,\mathrm{sh}\,\varphi - A - \frac{8h_0\pi^2\xi}{A}(B + \mathrm{sh}^2\,\varphi), \quad \text{(B22)}$$

and $X_3 = -Y_3 = -A\,\mathrm{sh}\,\varphi$, $T_3 = -A$.

B.4. *Summation procedure*

The two basic sums utilized in the summation procedure for the stresses due to considered periodic dislocation arrays are

$$\sum_{n=-\infty}^{\infty} \frac{1}{z^2 + (\eta - n)^2} = \frac{2\pi^2}{A\varphi}\,\mathrm{sh}\,\varphi, \quad \text{(B23)}$$

and

$$\sum_{n=-\infty}^{\infty} \frac{\eta-n}{z^2+(\eta-n)^2} = \frac{\pi}{A}\sin\psi. \tag{B24}$$

The following formulas are also used, which can be derived from eqn (B23) and (B24) by appropriate differentiation:

$$\sum_{n=-\infty}^{\infty} \frac{1}{[z^2+(\eta-n)^2]^2} = \frac{4\pi^4}{A^2\varphi^3}(A\,\mathrm{sh}\,\varphi+B\varphi) \tag{B25}$$

$$\sum_{n=-\infty}^{\infty} \frac{1}{[z^2+(\eta-n)^2]^3} = \frac{4\pi^6}{A^3\varphi^5}[3A(A\,\mathrm{sh}\,\varphi+B\varphi)-\varphi^2\,\mathrm{sh}\,\varphi(B-\sin^2\psi)], \tag{B26}$$

and

$$\sum_{n=-\infty}^{\infty} \frac{\eta-n}{[z^2+(\eta-n)^2]^2} = \frac{2\pi^3}{A^2\varphi}\sin\psi\,\mathrm{sh}\,\varphi \tag{B27}$$

$$\sum_{n=-\infty}^{\infty} \frac{\eta-n}{[z^2+(\eta-n)^2]^3} = \frac{2\pi^5}{A^3\varphi^3}\sin\psi[A\,\mathrm{sh}\,\varphi+\varphi(\mathrm{sh}^2\,\varphi+B)]. \tag{B28}$$

The abbreviations: $\varphi = 2\pi z$, $\psi = 2\pi\eta$, $A = \mathrm{ch}\,\varphi - \cos\psi$ and $B = \mathrm{ch}\,\varphi\cos\psi - 1$ were conveniently used.

APPENDIX C

When using a divergence theorem to calculate the elastic strain energy for a dislocation in an infinite bimaterial, or in a semi-infinite homogeneous body, the individual energy contributions from the cut, remote contour and core surface depend on a selected cut surface over which displacement discontinuity is imposed. However, the total strain energy is independent of a selected cut, since neither stress nor strain depends on such a selection. For dislocations in a homogeneous medium, this was discussed by Bullough and Foreman (1964), and Gavazza and Barnett (1975). The energy calculated from eqn (3), which implies displacement discontinuity along the horizontal cut, is given by eqn (4). However, if displacement discontinuity is imposed along the vertical cut, so that

$$E = -\frac{1}{2}b_x\int_\rho^R \sigma_x^{(1)}(h,y)\,\mathrm{d}y + E_R - E_\rho, \tag{C1}$$

the strain energy becomes

$$E = \frac{1}{2}k_1 b_x^2\left(\ln\frac{2h}{\rho} + k_3\ln\frac{R}{2h} + \frac{3}{2}k_2\right) + E_R - E_\rho. \tag{C2}$$

Therefore, the bracketed terms in eqns (4) and (C2) differ by k_2. The reason for this difference can be readily understood by considering horizontal equilibrium of a large block of material (1), shown in Fig. C1, i.e.

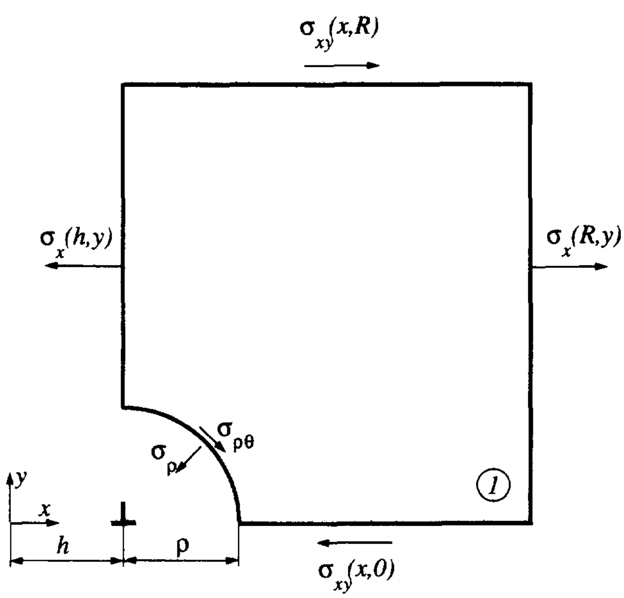

Fig. C1. A large square block of material (1) with excluded dislocation core segment of radius ρ. Indicated are the stress components that contribute to the balance of horizontal forces, leading to eqn (C4). Dislocation is at a distance h from the bimaterial interface along the y axis.

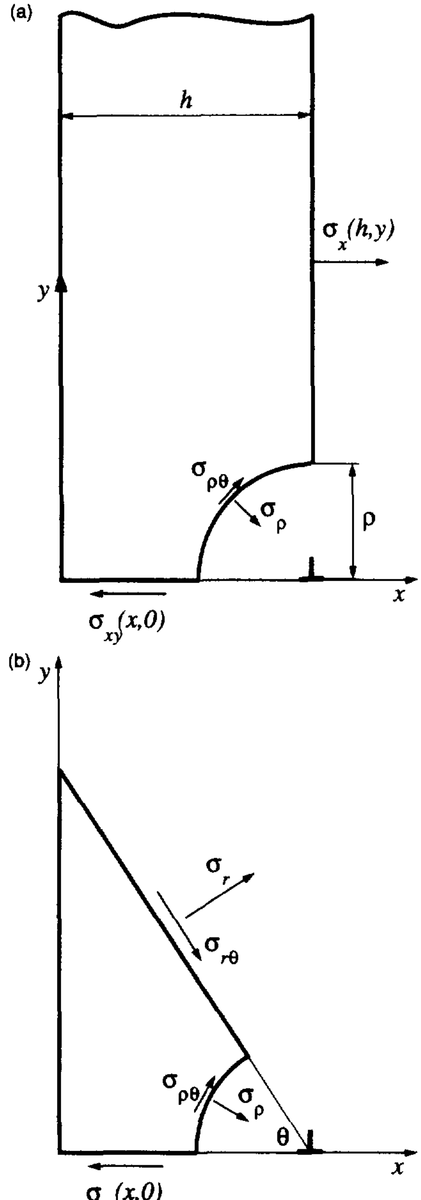

Fig. C2. (a) A semi-infinite strip with an excluded dislocation core segment of radius ρ. Dislocation is at a distance h from the free surface along the y axis. Indicated are the stress components that contribute to balance of the horizontal forces. (b) A quasi-triangular segment of a semi-infinite strip from (a).

$$\int_h^R \sigma_x^{(1)}(h,y)\,\mathrm{d}y+\int_{h+\rho}^R \sigma_{xy}^{(1)}(x,0)\,\mathrm{d}x=\int_0^R \sigma_x^{(1)}(R,y)\,\mathrm{d}y+\int_h^R \sigma_{xy}^{(1)}(x,R)\,\mathrm{d}x+\int_0^{\pi/2}(\sigma_{\rho\theta}\sin\theta-\sigma_\rho\cos\theta)\rho\,\mathrm{d}\theta. \quad \text{(C3)}$$

For a sufficiently small core radius ($\rho \ll h$), the dislocation core can be replaced with a cylindrical hole whose surface is subjected to tractions of an isolated dislocation in an infinite homogeneous medium, which are $\sigma_\rho = -k_1 b_x \sin\theta/\rho$ and $\sigma_{\rho\theta} = k_1 b_x \cos\theta/\rho$. Hence, by using eqns (A9) and (A11) for $\sigma_x^{(1)}(R,y)$ and $\sigma_{xy}^{(1)}(x,R)$, the integration gives

$$\int_h^R \sigma_x^{(1)}(h,y)\,\mathrm{d}y+\int_{h+\rho}^R \sigma_{xy}^{(1)}(x,0)\,\mathrm{d}x=-k_1k_2b_x. \quad \text{(C4)}$$

Thus, the energy difference $k_1k_2b_x^2/2$. If two materials are identical ($k_2 = 0$), the difference is equal to zero, and the respective energy contributions do not depend on a selected cut surface along which displacement discontinuity is imposed. if dislocation is near the free surface of a semi-infinite homogeneous body ($k_2 = -1$), the difference in cut contributions is $k_1b_x^2/2$. This can be obtained by an independent analysis, considering horizontal equilibrium of a semi-infinite strip near the free surface, with the excluded dislocation core segment [Fig. C2(a)]. The result is

$$\int_{\rho}^{\infty}\sigma_x(h,y)\,\mathrm{d}y-\int_0^{h-\rho}\sigma_{xy}(x,0)\,\mathrm{d}x = k_1 b_x, \tag{C5}$$

which is equal and opposite to the resulting horizontal force of the surface tractions over the considered core segment. More generally, from horizontal equilibrium of an isolated quasi-triangular region shown in Fig. C2(b), it follows that

$$\int_{\rho}^{h\sec\theta}(\sigma_{r\theta}\cos\theta+\sigma_r\sin\theta)\,\mathrm{d}s-\int_0^{h-\rho}\sigma_{xy}(x,0)\,\mathrm{d}x = \frac{1}{2}k_1 b_x(1-\cos 2\theta), \tag{C6}$$

which is equal and opposite to the resulting horizontal force over the core segment of arc-length θ. Therefore, the energy contributions calculated from the integrals along the horizontal cut and the cut inclined at an angle θ differ by $k_1 b_x^2(1-\cos 2\theta)/4$. Analogous conclusions apply for a dislocation with the Burgers vector parallel or arbitrarily inclined to the interface or the free surface. However, the total elastic strain energy E is independent of the cut surface, because the difference in the contributions from integrals along two different cut surfaces is exactly balanced by the difference in the contributions from the core surface. For example, the core contribution associated with the horizontal cut for a dislocation with the Burgers vector normal to the free surface in a semi-infinite body is $E_\rho = k_1 b_x^2(1-2\nu_1)/8(1-\nu_1)$. Since the core contribution associated with the vertical cut is $E_\rho = -k_1 b_x^2(3-2\nu_1)/8(1-\nu_1)$, the total strain energies are in both cases equal to

$$E = \frac{1}{2}k_1 b_x^2\left[\ln\frac{2h}{\rho}-\frac{3-4\nu}{4(1-\nu)}\right]. \tag{C7}$$

This is why seemingly different energy expressions for a dislocation near the free surface of a semi-infinite body, obtained by Willis *et al.* (1990; 1991) with the cut along the normal to the free surface, and Freund (1987; 1990) with the cut along an inclined (glide) plane, lead to the same total strain energy.

The energy core contributions associated with displacement discontinuity imposed at an angle $0 \leqslant \theta \leqslant 2\pi$ and the angle $\theta = 0$ are related through

$$E_\rho(\theta) = \frac{1}{2}\int_{\theta}^{\theta+2\pi}\mathbf{t}\cdot\mathbf{u}\rho\,\mathrm{d}\theta = E_\rho(0)+\frac{1}{2}\mathscr{F}_x(\theta)b_x, \tag{C8}$$

where

$$\mathscr{F}_x(\theta) = \int_0^{\theta}(\sigma_\rho\cos\theta-\sigma_{\rho\theta}\sin\theta)\rho\,\mathrm{d}\theta = -\frac{1}{2}k_1 b_x(1-\cos 2\theta) \tag{C9}$$

is the net horizontal force from the tractions over the core segment of arc-length θ. The second term on the right-hand side of eqn (C8) is the work of this force associated with the horizontal translation of the considered segment for amount b_x, imposed to change displacement discontinuity from the horizontal cut to an inclined cut at the angle θ. Hence

$$E_\rho(\theta) = \frac{1}{4}k_1 b_x^2\left[\cos 2\theta-\frac{1}{2(1-\nu_1)}\right]. \tag{C10}$$

More generally, for a dislocation with the Burgers vector $\{b_x, b_y\}$, the energy core contributions associated with the horizontal and inclined cuts are related through

$$E_\rho(\theta) = E_\rho(0)+\tfrac{1}{2}\mathscr{F}_x(\theta)b_x+\tfrac{1}{2}\mathscr{F}_y(\theta)b_y, \tag{C11}$$

where

$$\mathscr{F}_x(\theta) = \tfrac{1}{2}k_1[b_y\sin 2\theta-b_x(1-\cos 2\theta)] \tag{C12}$$

$$\mathscr{F}_y(\theta) = \tfrac{1}{2}k_1[b_x\sin 2\theta+b_y(1-\cos 2\theta)]. \tag{C13}$$

Therefore, in view of eqn (10) for $E_\rho(0)$, eqn (C11) gives

$$E_\rho(\theta) = \frac{1}{4}k_1\left[(b_x^2-b_y^2)\cos 2\theta+2b_x b_y\sin 2\theta-\frac{1}{2(1-\nu_1)}(b_x^2+b_y^2)\right]. \tag{C14}$$

If $b_x = b\cos\vartheta$ and $b_y = b\sin\vartheta$, eqn (C14) can be written as

$$E_\rho(\theta) = \frac{1}{4}k_1 b^2\left[\cos 2(\theta-\vartheta)-\frac{1}{2(1-\nu_1)}\right]. \tag{C15}$$

APPENDIX D

The strain energy expression derived in Section 3.2 can be obtained by an alternative procedure which does not require the use of the shear stress expression (24). Indeed, since σ_{xy} is the negative mixed derivative of the Airy stress function with respect to x and y coordinates, by superimposing the contributions from all dislocations in the wall, one has

$$\int_{h+\rho}^{R} \sigma_{xy}^{(1)}(x,0)\,\mathrm{d}x = \sum_{n=-\infty}^{\infty}\left[\frac{\partial\Phi^{(1)}}{\partial y}(h+\rho,-np) - \frac{\partial\Phi^{(1)}}{\partial y}(R,-np)\right], \tag{D1}$$

where, from eqn (A7),

$$\frac{\partial\Phi^{(1)}}{\partial y}(x,-np) = -k_1 b\left[\ln r_1 + \frac{n^2p^2}{r_1^2} + (k_3-1)\left(\ln r_2 + \frac{n^2p^2}{r_2^2}\right) - 2k_2hx\left(\frac{1}{r_2^2} - \frac{2n^2p^2}{r_2^4}\right) + \beta k_3\frac{(x+h)^2}{r_2^2}\right], \tag{D2}$$

with $r_1^2 = (x-h)^2 + n^2p^2$, and $r_2^2 = (x+h)^2 + n^2p^2$. Performing the requisite summations, it follows that

$$\int_{h+\rho}^{R} \sigma_{xy}^{(1)}(x,0)\,\mathrm{d}x = k_1 b\left\{\ln\frac{\operatorname{sh}\varphi_0}{\operatorname{sh}\rho_0} + \rho_0\coth\rho_0 + k_2\left(\varphi_0\coth\varphi_0 + \frac{\varphi_0^2}{2\operatorname{sh}^2\varphi_0}\right) + k_3\left[\beta\left(R_0 + \frac{\varphi_0}{2}\right) - \ln(2\operatorname{sh}\varphi_0)\right]\right\}, \tag{D3}$$

employing the same notation as in the body of the paper. This leads to eqn (30) of Section 3.2. In the procedure, the following result is helpful

$$\sum_{n=1}^{\infty} \ln\frac{z^2+n^2}{w^2+n^2} = \ln\frac{\operatorname{sh}\pi z}{\pi z} - \ln\frac{\operatorname{sh}\pi w}{\pi w}, \tag{D4}$$

which can be derived by using the representation of the hyperbolic sine function in the form of an infinite product

$$\operatorname{sh} z = z\prod_{n=1}^{\infty}\left(1 + \frac{z^2}{\pi^2 n^2}\right). \tag{D5}$$