Elastic energy of interaction of a point defect with a grain boundary

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Analytic expressions for the elastic energy of interaction of a point defect with a planar defect, a plane of dilatation, and half a plane of dilatation in a planar defect have been calculated. The implications with regard to segregation of impurities near high-angle grain boundaries are discussed.

I. INTRODUCTION

Segregation of solute atoms to or away from grain boundaries is of great interest from an experimental and theoretical point of view. Several different mechanisms should be differentiated for solute segregation at grain boundaries. Mechanisms for equilibrium segregation include the reduction of interfacial energy or the accommodation of excess strain from solutes which fit poorly in the lost material (either because of elastic or electronic mismatch). We shall not consider in this paper the problem of segregation to low-angle boundaries (misorientation angle less than 15°) which consist of arrays of discrete dislocations.

The purpose of this paper is to present the calculation of the strain energy of a point defect in the vicinity of a general high-angle grain boundary. Two models of the grain boundary are considered which may represent it at different stages of the segregation process.

The energy of interaction between a point defect and an interface has been studied in elasticity theory.[1,2] In an anisotropic crystal, the impurity sees the misoriented half-crystal in which it does not reside with average elastic constants different from those of the host half crystal. The calculation of the strain energy of a point defect near an interface between two crystals with different elastic constants leads to an interaction which decreases as the inverse of the cube of the distance. The impurity is attracted or repelled depending on the values of ratios of elastic constants in the two crystals.

We start by considering a stress-free purely planar grain boundary to consist of a core region of "bad" material sandwiched between two perfect crystals. By "bad" material we mean that the atomic structure of the core region is highly disorganized. The core region is therefore essentially a thin slab with elastic constants different from those of the two semi-infinite regions it connects. An A-B-A planar defect of this type may also describe a grain boundary wetted by some other phase.

In Sec. II, we review briefly the equations which permit the calculation of strain energies due to a distribution of body forces. The self-strain energy of a point defect in the vicinity of an A-B-A planar defect is reported in Sec. III. In Sec. IV, forces of dilatation are introduced in the planar defect. Solute atoms segregating in the core of the boundary could be sources of such forces of dilatation. The model of a stressed A-B-A planar defect may be a description of a grain boundary in a later stage of segregation. The elastic energy of interaction of a point defect with a single force of dilatation, a half plane of dilatation, and an infinite plane of dilatation in the planar defect are calculated. The conclusions drawn from this work are discussed in Sec. V.

II. ELASTIC ENERGY OF A DISTRIBUTION OF BODY FORCE

We denote by $\mathbf{F}$ a body force per unit volume. The strain energy associated with the introduction of the body force is given by[3]

$$U_s=\frac{1}{2}\sum_{\alpha,\beta}\int d^3X\int d^3X'\,F_\alpha(\mathbf{X})g^0_{\alpha\beta}(\mathbf{X},\mathbf{X}')F_\beta(\mathbf{X}')\ , \tag{1}$$

where $g^0_{\alpha\beta}(\mathbf{X},\mathbf{X}')$ is the Green function of the medium. When the medium has the translational symmetry perpendicular to the direction X_3, the Green function can be Fourier analyzed:

$$g^0_{\alpha\beta}(\mathbf{X},\mathbf{X}')=\int\frac{d^2K_\parallel}{(2\pi)^2}g^0_{\alpha\beta}(\mathbf{K}_\parallel|X_3,X_3')\times\exp[i\mathbf{K}_\parallel\cdot(\mathbf{X}_\parallel-\mathbf{X}_\parallel')]\ , \tag{2}$$

where $\mathbf{K}_\parallel$ and $\mathbf{X}_\parallel$ are both two-dimensional vectors with components $(K_1,K_2,0)$ and $(X_1,X_2,0)$.

In the case of a medium isotropic in planes perpendicular to X_3, the Green function can be expressed in terms of simpler coefficients by rotating the vector $\mathbf{K}_\parallel$ into a vector $(K_\parallel,0,0)$ with the transformation

$$S(\hat{K}_\parallel)=\begin{bmatrix}\hat{K}_1 & \hat{K}_2 & 0\\ -\hat{K}_2 & \hat{K}_1 & 0\\ 0 & 0 & 1\end{bmatrix}\quad\text{and}\quad \hat{K}_\alpha=K_\alpha/K_\parallel\quad(\alpha=1,2)\ . \tag{3}$$

The Green function is written in the form

$$g^0_{\alpha\beta}(\mathbf{K}_\parallel|X_3,X'_3)=\sum_{\mu,\nu} S^{-1}_{\alpha\mu}(\hat{K})g_{\alpha\beta}(K_\parallel|X_3,X'_3)S_{\nu\beta}(\hat{K}) \tag{4}$$

and the strain energy becomes

$$U_s=\tfrac{1}{2}\sum_{\mu,\nu}\int\frac{d^2K_\parallel}{(2\pi)^2}\int dX_3\int dX'_3\, f_\mu(\mathbf{K}_\parallel|X_3)\times g_{\mu\nu}(K_\parallel|X_3,X'_3)\times f^*_\nu(\mathbf{K}_\parallel|X'_3)\ , \tag{5}$$

where

$$f_\mu(\mathbf{K}_\parallel|X_3)=\sum_\alpha S_{\mu\alpha}(\hat{K}_\parallel)\int d^2X_\parallel\, F_\alpha(\mathbf{X})\exp(i\mathbf{K}_\parallel\cdot\mathbf{X}_\parallel)\ . \tag{6}$$

The $*$ in Eq. (5) denotes the complex conjugate.

Equation (1) permits the calculation of the strain energy due to the superposition of two body forces $\mathbf{F}^{(1)}(\mathbf{X}|\mathbf{X}^{(1)})$ and $\mathbf{F}^{(2)}(\mathbf{X}|\mathbf{X}^{(2)})$, where $\mathbf{X}^{(1)}$ and $\mathbf{X}^{(2)}$ are the positions of the two individual forces.

The total strain energy is the sum of the self-strain energies of the individual forces and the interaction strain energy.

After carrying out the same transformations on the interaction strain energy as those mentioned above, the interaction energy is given in Ref. 3 in the form

$$U_I(\mathbf{X}^{(1)},\mathbf{X}^{(2)})=\sum_{\mu,\nu}\int\frac{d^2K_\parallel}{(2\pi)^2}\int dX_3\int dX'_3\, f^{(1)}_\mu(\mathbf{K}_\parallel|X_3)\times g_{\mu\nu}(K_\parallel|X_3,X'_3)\times f^{(2)*}_\nu(\mathbf{K}_\parallel|X'_3)\ , \tag{7}$$

where

$$f^{(j)}_\mu(\mathbf{K}_\parallel|X_3)=\sum_\alpha S_{\mu\alpha}(\hat{K}_\parallel)\int d^2X_\parallel\, F^{(j)}_\alpha(\mathbf{X}|\mathbf{X}^{(j)})\times\exp(i\mathbf{K}_\parallel\cdot\mathbf{X}_\parallel),\quad j=1,2\ . \tag{8}$$

We must now specify the distributions of body force we use in this work to describe a point defect and a stressed high-angle grain boundary.

We represent a spherically symmetric point defect by the superposition of three mutually perpendicular double forces without moment centered at a point $\mathbf{X}_0$.

That is, $\mathbf{F}(\mathbf{X})$ is expressed as

$$F_\alpha(\mathbf{X})=-A_0\frac{\partial}{\partial X_\alpha}\delta(\mathbf{X}-\mathbf{X}_0),\quad \alpha=1,2,3 \tag{9}$$

where A_0 is a constant with the dimensions of force times length.

The $f_\mu(\mathbf{K}_\parallel|X_3)$'s of the symmetrical point defect defined in Eq. (6) are

$$f_1(\mathbf{K}_\parallel,X_3)=iA_0K^2_\parallel\delta(X_3-X_{03})\exp(i\mathbf{K}_\parallel\cdot\mathbf{X}^{(0)}_\parallel)\ , \tag{10a}$$

$$f_2(\mathbf{K}_\parallel,X_3)=0\ , \tag{10b}$$

$$f_3(\mathbf{K}_\parallel,X_3)=-A_0\frac{d}{dX_3}\delta(X_3-X_{03})\exp(i\mathbf{K}_\parallel\cdot\mathbf{X}^{(0)}_\parallel)\ , \tag{10c}$$

where $\mathbf{X}^{(0)}_\parallel$ is the position of the point defect in a plane perpendicular to X_3.

Easy relaxation along the boundary plane of the forces corresponding to point defects segregating at high-angle grain boundaries results in the introduction of forces of dilatations in the core of the boundary perpendicular to the boundary plane. We represent the dilatation at every position $X^{(B)}_\parallel$ on the plane $X_3=0$ by a single double force without moment of the type

$$F_1=0\ , \tag{11a}$$

$$F_2=0\ , \tag{11b}$$

$$F_3=-A\frac{\partial}{\partial X_3}\delta(\mathbf{X}_\parallel-\mathbf{X}^{(B)}_\parallel)\delta(X_3)\ , \tag{11c}$$

where A is again a constant with the dimensions of force times length.

This force after transformation becomes

$$f_1(\mathbf{K}_\parallel,X_3)=0\ , \tag{12a}$$

$$f_2(\mathbf{K}_\parallel,X_3)=0\ , \tag{12b}$$

$$f_3(\mathbf{K}_\parallel,X_3)=-A\frac{\partial}{\partial X_3}\delta(X_3)\exp(i\mathbf{K}_\parallel\cdot\mathbf{X}^{(B)}_\parallel)\ . \tag{12c}$$

III. SELF-STRAIN ENERGY OF A POINT DEFECT NEAR A PLANAR DEFECT

The planar defect is constituted of a slab B sandwiched between two semi-infinite media A. The thickness of the slab centered on $X_3=0$ is $2a$. The media A and B are assumed to to be isotropic with elastic constants C_{11},C_{44} and C'_{11},C'_{44}, respectively.

The Green function g of an A-B-A planar defect is the sum of the Green function of an infinite medium, G^∞, and the contribution of the interfaces between media A and B, $G=g-G^\infty$. The excess strain energy of the point defect due to the slab is given by Eq. (5) where one substitutes G for g. The point defect is located in the left semi-infinite medium at a distance X_{03} from the center of the slab.

It follows from Eqs. (5) and (10) that the strain energy is independent of $\mathbf{X}^{(0)}_\parallel$. Furthermore, only the sagittal elements of the Green function are necessary for the calculation of the strain energy of a spherically symmetric point defect. The sagittal part of the interfacial contribution to the Green function, $G(K_\parallel|X_3X'_3)$ of the A-B-A sandwich in the region $X_3<-a$ and $X'_3<-a$, is given in the Appendix. The excess strain energy is calculated in the form

$$U_s=\frac{A_0^2}{8\pi C^2_\parallel}\int_0^{K_D}dK_\parallel\, K_\parallel e^{-2K_\parallel|X_{03}|}\phi(K_\parallel)\ , \tag{13}$$

where K_D is the radius of the Debye circle throughout which the integration over $K_\parallel$ is carried out. Such a cutoff arises from the discrete nature of the lattices. $\phi(K_\parallel)$ is defined as $\frac{1}{2}(A^S+A^A+H^S+H^A)$, where the $A^{S,A}$ and $H^{S,A}$ are given in the Appendix. We note that in the limit $C'_{44}=0$,

$$\phi(K_\parallel)=-4K_\parallel\frac{C_{44}C_{11}}{(C_{11}-C_{44})}$$

and

$$U_s=-\frac{A_0^2}{16\pi}\frac{C_{44}}{C_{11}(C_{11}-C_{44})}\frac{1}{|X_{03}|^3}I_2(\xi)\ , \tag{14}$$

where we use the notation

$$I_n(\xi)=\int_0^\xi du\, u^n e^{-u},\quad \xi=2K_\parallel|X_{03}|\ . \tag{15}$$

This is the excess energy of a point defect in the vicinity of a free surface.[3]

In the limit of a very thin slab, that is $(aK_\parallel)\ll 1$, the function $\phi(K_\parallel)$ simplifies to

$$\phi(K_\parallel)=8aK_\parallel^2C_{44}\frac{\nu'}{1+\nu}\left[1-\frac{h_{11}}{h_{44}^2}\frac{(1+\nu')}{(1+\nu)}\right]\ , \tag{16}$$

where we define $\nu=C_{44}/C_{11}$, $\nu'=C'_{44}/C'_{11}$, $h_{11}=C'_{11}/C_{11}$, and $h_{44}=C'_{44}/C_{44}$. The excess strain energy of the point defect reduces to

$$U_s=\frac{A_0^2}{16\pi C_{11}}\frac{\nu\nu'}{(1+\nu)}\frac{a}{|X_{03}|^4}\left[1-\frac{h_{11}}{h_{44}^2}\frac{(1+\nu')}{(1+\nu)}\right]I_3(\xi)\ . \tag{17}$$

From the simpler expression, we note that the energy can be either positive or negative, depending upon the values of the ratios of elastic constants of the media A and B. In particular, a point defect of the kind considered here is attracted or repelled by the planar defect when $C'_{44}\ll C_{44}$ or $C'_{44}\gg C_{44}$, respectively.

IV. INTERACTION BETWEEN A POINT DEFECT AND A STRESSED PLANAR DEFECT

We now turn to a discussion of the strain energy of interaction of a point defect and forces of dilatation in the planar defect.

The A-B-A planar defect is the same as in Sec. III.

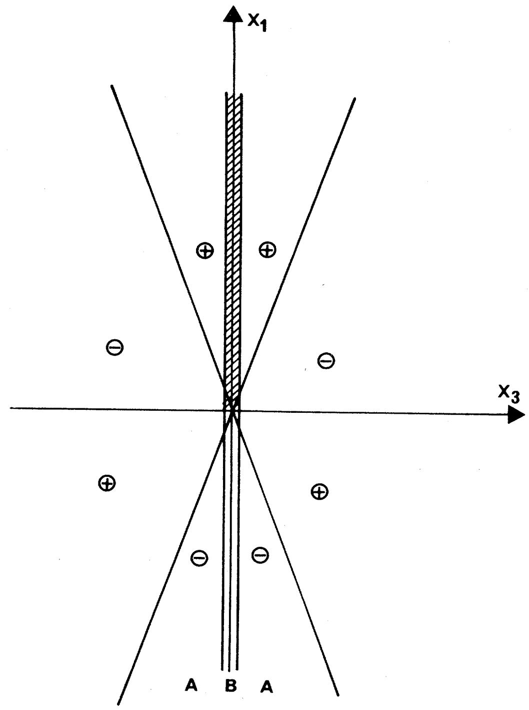

FIG. 1. Domains of variation of sign of the interaction energy of a point defect and a plane of dilatation in a planar defect when $AA_0<0$. The dashed region corresponds to the half-plane of dilatation.

The forces of dilatation are single double forces of the type given by Eqs. (11). We calculate initially the energy of interaction of a spherically symmetric point defect located at $(X_\parallel^{(0)}, X_{03}>a)$ and a single double force located at $(X_\parallel^{(B)}, X_3^B=0)$. For the sake of simplicity, we carry out the integration of Eq. (7) in the limit of a very thin slab, that is, in the limit $(aK_\parallel)\ll 1$. We give in the Appendix expressions for the Green functions, $g(K_\parallel|X_3,X'_3|)$ of a thin planar defect when X_3 is in the slab and X'_3 is in the right semi-infinite medium. The integration of Eq. (7) yields the result that

$$U_I=\frac{-A_0A}{4\pi C_{44}}\left[(1-2\nu')\frac{2}{(R_\parallel^2+X_{03}^2)^{3/2}}P_2\left[\frac{X_{03}}{(R_\parallel^2+X_{03}^2)^{1/2}}\right]-\left[\frac{2C_{44}}{C'_{11}}+(1-2\nu')\right](1-\nu)\frac{6X_{03}}{(R_\parallel^2+X_{03}^2)^2}P_3\left[\frac{X_{03}}{(R_\parallel^2+X_{03}^2)^{1/2}}\right]\right]\ , \tag{18}$$

where $\mathbf{R}_\parallel=\mathbf{X}_\parallel^{(0)}-\mathbf{X}_\parallel^{(B)}$. $P_n(X)$ is the nth Legendre polynomial.

The total strain energy of interaction of the point defect with an infinite plane of dilatation is obtained by integration of U_I over all $R_\parallel$. This energy is found to vanish due to the translational symmetry of the plane of dilatation. The strain energy of a point defect with the half plane of dilatation $(X_1^{(B)}\ge 0)$ is nonzero and obtained in the form

$$U_{I\,1/2}=-\frac{A_0A}{2\pi C_{44}}\frac{X_{01}}{X_{01}^2+X_{03}^2}\times\left[(1-2\nu')-\left[\frac{2C_{44}}{C'_{11}}+(1-2\nu')\right]\times(1-\nu)\frac{2X_{03}^2}{(X_{01}^2+X_{03}^2)^2}\right]\ . \tag{19}$$

This energy is long ranged and varies as the inverse of the distance X_{01} of the point defect to the tip of the half-plane of dilatation and as the inverse of the square of the distance X_{03} from the planar defect.

In the limit $X_{01} \rightarrow +\infty$, the energy vanishes as the point defect sees an infinite plane of dilatation.

Equation (19) simplifies to

$$U_{I\,1/2}^{(X_{03}=0)} = -\frac{A_0 A}{2\pi C_{44}}(1-2\nu')\frac{1}{X_{01}} \tag{20}$$

when the point defect is located very near the core of the planar defect.

V. CONCLUSION

The excess energy of a spherically symmetry point defect in the neighborhood of a planar defect is short ranged and varies as the inverse fourth power of the distance of the defect from the planar defect. This energy can be either attractive or repulsive, depending on the elastic constants of the core region and of the semi-infinite regions.

The interaction energy of one point defect with an infinite plane of dilatation in the planar defect is zero. However, the elastic energy of interaction of the point defect with half a plane of dilatation in the planar defect is long ranged and varies as the inverse of the distance from the tip of the plane and the inverse of the square of the distance from the planar defect.

The sign of this latter energy varies spatially (Fig. 1). The extent of these variations is controlled by the values of the elastic constants in both media A and B. Moreover, the energy of interaction is attractive of repulsive depending on whether the double forces modeling the point defect and stressed planar defect are dilatational or contractive forces.

Before reaching a complete understanding of the segregation process, one has to evaluate the other contributions to the interaction energy between one point defect and the grain boundary, such as the electronic interactions, space charge effect in an ionic crystal and semiconductors, etc. The electronic interaction of a heterovalent impurity with a boundary in a crystal of normal metal has been calculated via pair interactions deduced from pseudopotentials.[4] The interaction has been found to decrease as the inverse of the square of the distance.

The electronic binding energy can be sizable when compared with the excess strain energy. However, the elastic contribution to the interaction energy between a defect and a stressed grain boundary in a metal is expected to be one of the leading ones.

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APPENDIX

We give in this appendix the sagittal elements of the static Green function $g_{\alpha\beta}(K_\parallel|X_3,X_3')$ of an A-B-A planar defect. The interface response theory of continuous materials[5] has been applied to the determination of the Green function of a composite material composed of an isotropic thin slab with elastic constants C_{11}',C_{44}', sandwiched between two semi-infinite regions with elastic constants C_{11},C_{44}. The planar interfaces are located at $X_3=-a$ and $X_3=+a$.

The Green function $g(X,X')$ at any two space points (X,X') in the space of the composite D is given by

$$\begin{aligned} g(DD) = {} & G(DD) - G(DM)G^{-1}(MM)G(MD) \\ & + G(DM)G^{-1}(MM)g(MM)G^{-1}(MM)G(MD) \,, \end{aligned} \tag{A1}$$

where M means that X or X' is limited to the domain of interfaces. $G(X,X')$ is the Green function of an infinite medium and $g(MM)$ is the interface response function of the composite.

The interface response function $g_i(MM)$ of every continuous subsystem i constituting the composite is determined by application of the universal equation of the interface response theory to the space M_i of the interfaces of i:

$$g_i(X,X') + \int dX''\, g_i(X,X'')A_i(X'',X') = G_i(X,X') \,, \quad \text{with } X,X',X'' \in M_i \,. \tag{A2}$$

The interface response operator A_i is defined in continuous media as $V_i G_i$, where V_i is a cleavage operator which creates out of an infinite medium the element i with its interface. The cleavage operator in elasticity theory has been given in Ref. 5. The planar defect has mirror symmetry. It proves more convenient to express all response functions in terms of symmetrical (S) and antisymmetrical (A) states.[6]

The transformation matrix

$$T = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & -1 & 0 \\ 0 & -1 & 0 & 1 \end{bmatrix}$$

permits the passage between the original state and the symmetrized states of the sagittal elements of the Green function. In the symmetrical and antisymmetrical states, there is separation of the response function in diagonal blocks.

The interface response function of the A-B-A sandwich is obtained in the form

$$\left.\begin{matrix} g_{11}^{A}(MM) \\ g_{11}^{A}(MM) \end{matrix}\right\} = \left\{\begin{matrix} (D^S)^{-1} \\ (D^A)^{-1} \end{matrix}\right\} \times \left[\frac{\alpha}{2} + \left\{\begin{matrix} C^S\cosh^2(aK_\parallel) \\ C^A\sinh^2(aK_\parallel) \end{matrix}\right\}\right] \,, \tag{A3a}$$

$$g_{13}^{S,A}(MM) = \frac{-i}{D^{S,A}}E^{S,A} \,, \tag{A3b}$$

$$g_{31}^{S,A}(MM)=\frac{i}{D^{S,A}}E^{S,A}\ , \tag{A3c}$$

$$\left.\begin{matrix} g_{33}^{S}(MM) \\ g_{33}^{A}(MM)\end{matrix}\right\}=\left\{\begin{matrix}(D^S)^{-1}\\ (D^A)^{-1}\end{matrix}\right\}\times\left[\frac{\alpha}{2}+\left\{\begin{matrix} C^S\sinh^2(aK_\parallel)\\ C^A\cosh^2(aK_\parallel)\end{matrix}\right\}\right]\ , \tag{A3d}$$

where

$$D^{S,A}=\frac{\alpha^2}{4}+\frac{\alpha}{2}C^{S,A}\cosh(2aK_\parallel)-(E^{S,A})^2+\frac{(C^{S,A})^2}{4}[\cosh^2(2aK_\parallel)-1]\ , \tag{A4}$$

$$C^{S,A}=\frac{\pm 2C'_{44}K_\parallel}{aK_\parallel(1-\nu')+\frac{1}{2}(1+\nu')\sinh(2aK_\parallel)}\ , \tag{A5}$$

$$E^{S,A}=\frac{\alpha\nu}{2}\pm C^{S,A}\left[(1-\nu')aK_0+\frac{\nu'}{2}\sinh(2aK_\parallel)\right]\ , \tag{A6}$$

$$\alpha=-\frac{4K_\parallel C_{44}}{1+\nu}\ ,$$

$$\nu=\frac{C_{44}}{C_{11}}\quad\text{and}\quad \nu'=\frac{C'_{44}}{C'_{11}}\ .$$

The Green function $G^\infty(K_\parallel|X_3,X'_3)$ of an infinite isotropic medium has been calculated,[3]

$$G_{11}^\infty(K_\parallel|X_3,X'_3)=\frac{1}{4K_\parallel C_{44}}[-(1+\nu)+K_\parallel(1-\nu)|X_3-X'_3|]\exp(-K_\parallel|X_3-X'_3|)\ , \tag{A7a}$$

$$G_{13}^\infty(K_\parallel|X_3,X'_3)=G_{31}(K_\parallel|X_3,X'_3)=\frac{iK_\parallel}{4K_\parallel C_{44}}(1-\nu)(X_3-X'_3)\exp(-K_\parallel|X_3-X'_3|)\ , \tag{A7b}$$

$$G_{33}^\infty(K_\parallel|X_3,X'_3)=\frac{-1}{4K_\parallel C_{44}}[(1+\nu)+K_\parallel(1-\nu)|X_3-X'_3|]\exp(-K_\parallel|X_3-X'_3|)\ . \tag{A7c}$$

We report in this Appendix the Green function in two regions of the A-B-A composite.

(1) X_3 and X'_3 in the left semi-infinite medium. The contribution of the interfaces to the Green's function $G(DD)=g(DD)-G^\infty(DD)$ is given in the symmetrical-antisymmetrical base in the form

$$G_{11}^{S,A}=A^{S,A}(a_0a'_0+b_0b'_0)+B^{S,A}(a_0a'_0-b_0b'_0)+iC^{S,A}(b_0a'_0-a_0b'_0)\ , \tag{A8a}$$

$$G_{13}^{S,A}=A^{S,A}(a_0b'_0+b_0d'_0)+B^{S,A}(a_0b'_0-b_0d'_0)-iC^{S,A}(a_0d'_0-b_0b'_0)\ , \tag{A8b}$$

$$G_{31}^{S,A}=A^{S,A}(a'_0b_0+b'_0d_0)+B^{S,A}(a'_0b_0-b'_0d_0)-iC^{S,A}(a'_0d_0-b'_0b_0)\ , \tag{A8c}$$

$$G_{33}^{S,A}=A^{S,A}(b_0b'_0+d_0d'_0)+B^{S,A}(b_0b'_0-d_0d'_0)+iC^{S,A}(d_0b'_0-b_0d'_0)\ , \tag{A8d}$$

where

$$A^{S,A}=\frac{\alpha^3+\alpha^2C^{S,A}\cosh(2aK_\parallel)-2\alpha D^{S,A}}{2D^{S,A}} \tag{A9}$$

$$B^S=+\frac{\alpha^2C^S}{2D^S},\quad B^A=-\frac{\alpha^2C^A}{2D^A}\ , \tag{A10}$$

$$C^{S,A}=\frac{\alpha^2E^{S,A}}{D^{S,A}}\ , \tag{A11}$$

and

$$a_0=G_{11}^\infty(X_3,0)\ ,$$

$$a'_0=G_{11}^\infty(0,X'_3)\ ,$$

$$b_0=G_{13}^\infty(X_3,0)\ ,$$

$$b'_0=G_{13}^\infty(0,X'_3)\ ,$$

$$d_0=G_{33}^\infty(X_3,0)\ ,$$

$$d'_0=G_{33}^\infty(0,X'_3)\ .$$

We note that in the limit $C'_{44}=0$, G simplifies to the interfacial contribution to the Green function of a semi-infinite medium.[3]

(2) X_3 in the right semi-infinite medium and X'_3 in the slab. In this case

$$G^\infty(DD)-G^\infty(DM)G^{-1}(MM)G^\infty(MD)=0$$

and we give the Green function in the limit $aK_\parallel \ll 1$:

$$g_{11}^S(K_\parallel|X_3,X'_3)=\alpha P_{11}^S\ ,$$

$$g_{13}^S(K_\parallel|X_3,X'_3)=\alpha\frac{X'_3}{a}P_{13}^S\ ,$$

$$g_{31}^S(K_\parallel|X_3,X'_3)=\alpha P_{31}^S\ ,$$

$$g_{33}^S(K_\parallel|X_{3,X'_3})=\alpha\frac{X'_3}{a}P_{33}^S\ ,$$

and

$$g_{11}^A(K_\parallel|X_3,X'_3)=\alpha\frac{X'_3}{a}P_{11}^A\ ,$$

$$g_{13}^A(K_\parallel|X_3,X'_3)=\alpha P_{13}^A\ ,$$

$$g_{31}^A(K_\parallel|X_3,X'_3)=\alpha\frac{X'_3}{a}P_{31}^A\ ,$$

$$g_{33}^A(K_\parallel|X_3,X'_3)=\alpha P_{33}^A\ ,$$

where

$$P_{11}^{S,A}=a_0\tilde{g}\,_{11}^{S,A}(MM)-b_0\tilde{g}\,_{31}^{S,A}(MM)\ ,$$

$$P_{13}^{S,A}=a_0\tilde{g}\,_{13}^{S,A}(MM)-b_0\tilde{g}\,_{33}^{S,A}(MM)\ ,$$

$$P_{31}^{S,A}=-b_0\tilde{g}\,_{11}^{S,A}(MM)+d_0\tilde{g}\,_{31}^{S,A}(MM)\ ,$$

$$P_{33}^{S,A}=-b_0\tilde{g}\,_{13}^{S,A}(MM)+d_0\tilde{g}\,_{33}^{S,A}(MM)\ .$$

The $\tilde{g}(MM)$ are the limits to first order of $g(MM)$ when $aK_{\parallel}\ll 1$.

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