# Elastic continuum theory of interface-atom mean-square displacements

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(Received 7 September 1976)

The mean-square displacements of particles near an interface between two different isotropic elastic continua are calculated for the first time. A Green's-function method was used in the high-temperature limit. The dependence of the mean-square displacements on distance from the interface is exhibited explicitly.

## I. INTRODUCTION

Extensive experimental[1] and theoretical[2] investigations of surface-atom mean-square displacements (MSD) have been carried out during the last few years. The experimental values can be obtained by low-energy electron diffraction, scattering of atoms,[3] or Mössbauer effect.[4] These techniques provide the atom MSD for clean surfaces as well as for surfaces covered with an adsorbed monolayer. One can expect that the atom MSD of surfaces covered with several monolayers will also be measured. The atom MSD near an interface between two solids can be measured qualitatively in this way, and may be measured quantitatively by more sophisticated techniques.

In the present paper, we study for the first time the MSD of particles near an interface between two different solids. We use an approach based on the Green's functions for two semi-infinite isotropic elastic media bounded by a planar interface. This approach[5] was used previously to calculate the surface-atom MSD as function of distance from the surface in the high-temperature limit. The values at the interface are obtained here in a way similar to that used for the surface.[5] We find in the present case that the difference between the interface and the bulk MSD becomes inversely proportional to the distance to the interface. This behavior was also obtained for the difference between the free surface and the bulk MSD.[5-7]

The necessary interface Green's functions have already been used for the calculation of the interface specific heat at low temperatures.[8] We will derive them in Sec. II. Then, (Sec. III) we will derive the atom MSD for atoms near an interface.

## II. INTERFACE GREEN'S FUNCTIONS

We consider now two different elastic isotropic media 1 and 2 occupying, respectively, the half-spaces $x_3>0$ and $x_3<0$. We need to know the Green's function $\vec{U}$ for the two crystals connected by this planar interface. The procedure is similar to the one used[9] for the surface. Let us first introduce the Green's function for crystal 1 which, inside the crystal, satisfies the equation

$$\sum_{\mu}\left(\delta_{\alpha\mu}\omega^2+\frac{1}{\rho}\sum_{\beta\nu}C_{\alpha\beta\mu\nu}\frac{\partial^2}{\partial x_\beta\,\partial x_\nu}\right)U_{\mu\gamma}(\vec{x},\vec{x}';\omega)=\delta_{\alpha\gamma}\delta(\vec{x}-\vec{x}'),\qquad(2.1)$$

where $C_{\alpha\beta\mu\nu}$ are the position-independent elastic moduli of the material, $\rho$ is the mass density, $\omega$ is the frequency of the time-dependent elastic displacement field in the medium, and $\alpha,\beta,\mu,\nu$ are the Cartesian indices $x$, $y$, or $z$. For an isotropic crystal, the $C_{\alpha\beta\mu\nu}$ are functions of the more usual elastic constants $C_{11}$, $C_{44}$, and $C_{12}=C_{11}-2C_{44}$.

The equation satisfied by the Green's function for crystal 2 is obtained from the one above by changing $\rho$ and $C_{\alpha\beta\mu\nu}$, respectively, to $\rho'$ and $C'_{\alpha\beta\mu\nu}$:

$$\sum_{\mu}\left(\delta_{\alpha\mu}\omega^2+\frac{1}{\rho'}\sum_{\beta\nu}C'_{\alpha\beta\mu\nu}\frac{\partial^2}{\partial x_\beta\,\partial x_\nu}\right)U_{\mu\gamma}(\vec{x},\vec{x}';\omega)=\delta_{\alpha\gamma}\delta(\vec{x}-\vec{x}').\qquad(2.2)$$

In order to obtain the Green's function $\vec{U}$ for the two crystals connected by a planar surface, we have to solve Eqs. (2.1) and (2.2) subject to the boundary conditions at $x_3=0$:

$$\sum_{\mu\nu} C_{\alpha z\mu\nu} \frac{\partial}{\partial x_\nu} U_{\mu\beta}(\vec{x}, \vec{x}'; \omega)\Big|_{x_3=+0} = \sum_{\mu\nu} C'_{\alpha z\mu\nu} \frac{\partial}{\partial x_\nu} U_{\mu\beta}(\vec{x}, \vec{x}'; \omega)\Big|_{x_3=-0}, \quad (2.3)$$

$$U_{\alpha\beta}(\vec{x}, \vec{x}'; \omega)\,|_{x_3=+0} = U_{\alpha\beta}(\vec{x}, \vec{x}'; \omega)\,|_{x_3=-0}. \quad (2.4)$$

Condition (2.3) comes from the continuity of the stresses across the interface and condition (2.4) from the continuity of the displacements. As a consequence of the symmetry of translation parallel to the interface, the Green's function $\vec{U}$ can be Fourier analyzed in the following manner:

$$U_{\alpha\beta}(\vec{x}, \vec{x}'; \omega) = \int \frac{d^2k}{(2\pi)^2} e^{i\vec{k}(\vec{x}_\parallel - \vec{x}'_\parallel)} d_{\alpha\beta}(\vec{k}\omega\,|x_3 x'_3), \quad (2.5)$$

where $\vec{x}_\parallel$ and $\vec{k}$ are both two-dimensional vectors with components $(x_1, x_2, 0)$ and $(k_1, k_2, 0) \equiv k(\cos\varphi, \sin\varphi, 0)$, respectively. We then use the isotropy of the medium in the plane $x_3 = 0$ and carry out a similarity transformation on our set of equations with respect to a matrix $\vec{S}(\vec{k})$ which rotates the vector $\vec{k}$ into the vector $(k, 0, 0)$:

$$\vec{S}(\vec{k}) = \begin{pmatrix} \cos\varphi & \sin\varphi & 0 \\ -\sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

In this transformation $\vec{d}$ is transformed into $\vec{g}$ and the Eqs. (2.1) and (2.2) can be written in the following matrix form[9]:

$$\begin{bmatrix} \omega^2 + \frac{1}{\rho}\left(C_{44}\frac{d^2}{dx_3^2} - C_{11}k^2\right) & 0 & \frac{i}{\rho}(C_{12}+C_{44})k\frac{d}{dx_3} \\ 0 & \omega^2 + \frac{C_{44}}{\rho}\left(\frac{d^2}{dx_3^2} - k^2\right) & 0 \\ \frac{i}{\rho}(C_{12}+C_{44})k\frac{d}{dx_3} & 0 & \omega^2 + \frac{1}{\rho}\left(C_{11}\frac{d^2}{dx_3^2} - C_{44}k^2\right) \end{bmatrix} \begin{pmatrix} g_{xx} & g_{xy} & g_{xz} \\ g_{yx} & g_{yy} & g_{yz} \\ g_{zx} & g_{zy} & g_{zz} \end{pmatrix}$$

$$= \delta(x_3 - x'_3) \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad (2.6)$$

An analogous equation is obtained also for medium 2. The boundary conditions (2.3) and (2.4) become

$$C_{44}\left(\frac{dg_{x\alpha}}{dx_3} + ikg_{z\alpha}\right)_{x_3=+0} = C'_{44}\left(\frac{dg_{x\alpha}}{dx_3} + ikg_{z\alpha}\right)_{x_3=-0}, \quad \left(C_{44}\frac{dg_{y\alpha}}{dx_3}\right)_{x_3=+0} = \left(C'_{44}\frac{dg_{y\alpha}}{dx_3}\right)_{x_3=-0}, \quad (2.7)$$

$$\left(i(C_{12}+C_{44})kg_{x\alpha} + C_{11}\frac{dg_{z\alpha}}{dx_3}\right)_{x_3=+0} = \left(i(C'_{12}+C'_{44})kg_{x\alpha} + C'_{11}\frac{dg_{z\alpha}}{dx_3}\right)_{x_3=-0}, \text{ and } (g_{\alpha\beta})_{x_3=+0} = (g_{\alpha\beta})_{x_3=-0}. \quad (2.8)$$

From these equations, one sees that, as for a semi-infinite crystal,[9] one has here also

$$g_{y\alpha} = g_{\alpha y} = 0, \quad \alpha = x \text{ or } z.$$

One can then calculate separately $g_{yy}$, $\{g_{xx}, g_{zx}\}$, and $\{g_{xz}, g_{zz}\}$. As an example, let us describe briefly the calculation of $\{g_{xx}, g_{zx}\}$.

In medium 1, one has from Eq. (2.6):

$$\left(\omega^2 - \frac{C_{11}}{\rho}k^2 + \frac{C_{44}}{\rho}\frac{d^2}{dx_3^2}\right)g_{xx} + \frac{i}{\rho}(C_{12}+C_{44})k\frac{dg_{zx}}{dx_3} = 0, \quad (2.9a)$$

$$\frac{i}{\rho}(C_{12}+C_{44})k\frac{dg_{xx}}{dx_3} + \left(\omega^2 - \frac{C_{44}}{\rho}k^2 + \frac{C_{11}}{\rho}\frac{d^2}{dx_3^2}\right)g_{zx} = 0. \quad (2.9b)$$

Eliminating $g_{zx}$ between the two Eqs. (2.9), we obtain a new differential equation for $g_{xx}$:

$$\left(\frac{d^2}{dx_3^2} - \alpha_t^2\right)\left(\frac{d^2}{dx_3^2} - \alpha_l^2\right)g_{xx} = \left(\frac{1}{C_t^2}\frac{d^2}{dx_3^2} - \frac{\alpha_t^2}{C_l^2}\right)\delta(x_3 - x'_3), \quad (2.10)$$

where

$$\alpha_t^2 = k^2 - \omega^2/C_t^2, \quad \alpha_l^2 = k^2 - \omega^2/C_l^2. \quad (2.11)$$

$C_t = (C_{44}/\rho)^{1/2}$ and $C_l = (C_{11}/\rho)^{1/2}$ are, respectively, the transverse and longitudinal speeds of sound in medium 1. The general solution of Eq. (2.10) can be written

$$g_{xx} = g^0_{xx} + A_t e^{-\alpha_t x_3} + A_l e^{-\alpha_l x_3}, \quad (2.12a)$$

where $g^0_{xx}$ is a particular solution of Eq. (2.10) giving the bulk Green's function

$$g^0_{xx}(k,\omega\,|x_3,x_3') = -\frac{k^2}{2\alpha_l\omega^2}\left(e^{-\alpha_l|x_3-x_3'|}-\frac{\alpha_l\alpha_t}{k^2}e^{-\alpha_t|x_3-x_3'|}\right).$$

In the same manner, one has in medium 1

$$g_{zx} = g^0_{zx} + B_t e^{-\alpha_t i x_3} + B_l e^{-\alpha_l i x_3}, \tag{2.12b}$$

with

$$g^0_{zx}(k\omega\,|x_3,x_3') = (ik/2\omega^2)\,\mathrm{sgn}(x_3-x_3')(e^{-\alpha_t|x_3-x_3'|}-e^{-\alpha_l|x_3-x_3'|}).$$

As a matter of fact, the coefficients $A_t$, $A_l$, $B_t$, and $B_l$ are not independent and with the help of Eqs. (2.9) one can obtain, for example, $B_t$ and $B_l$ as functions of $A_t$ and $A_l$ (Ref. 9);

$$B_t = i(k/\alpha_t)A_t, \quad B_l = i(\alpha_l/k)A_l. \tag{2.13}$$

In medium 2, one has in the same way

$$g_{xx} = g^0_{xx} + A'_t e^{\alpha'_t i x_3} + A'_l e^{\alpha'_l i x_3},$$

$$g_{zx} = g^0_{zx} + B'_t e^{\alpha'_t i x_3} + B'_l e^{\alpha'_l i x_3},$$

where $\alpha'_t$ and $\alpha'_l$, $g^0_{xx}$, and $g^0_{zx}$ are defined as in Eqs. (2.11) but with the parameters of medium 2. Here also $B'_t$ and $B'_l$ can be obtained as functions of $A'_t$ and $A'_l$.

Finally the four boundary conditions for $g_{xx}$ and $g_{zx}$ [Eqs. (2.7) and (2.8)] give a system of four linear equations with four unknowns $A_t$, $A_l$, $A'_t$, and $A'_l$. We write it in the matrix form

$$\vec{H}\begin{bmatrix}A_t\\A_l\\A'_t\\A'_l\end{bmatrix} = \vec{K}\begin{bmatrix}e^{-\alpha_t|x'_3|}\\e^{-\alpha_l|x'_3|}\\e^{-\alpha'_t|x'_3|}\\e^{-\alpha'_l|x'_3|}\end{bmatrix}, \tag{2.14}$$

where

$$\vec{H} = \begin{bmatrix} -C_{44}(\alpha_t^2+k^2)/\alpha_t & -2C_{44}\alpha_l & -C'_{44}(\alpha_t'^2+k^2)/\alpha'_t & -2C'_{44}\alpha'_l \\ -2iC_{44}k & -iC_{44}(\alpha_l^2+k^2)/k & 2iC'_{44}k & iC'_{44}(\alpha_t'^2+k^2)/k \\ 1 & 1 & -1 & -1 \\ ik/\alpha_t & i\alpha_l/k & ik/\alpha'_t & i\alpha'_l/k \end{bmatrix}, \tag{2.15}$$

and

$$\vec{K} = \begin{bmatrix} -C_{44}\frac{k^2+\alpha_t^2}{2\omega^2}\,\mathrm{sgn}x'_3 & C_{44}\frac{k^2}{\omega^2}\,\mathrm{sgn}x'_3 & C_{44}\frac{k^2+\alpha_t'^2}{2\omega^2}\,\mathrm{sgn}x'_3 & -C'_{44}\frac{k^2}{\omega^2}\,\mathrm{sgn}x'_3 \\ iC_{44}\frac{k\alpha_t}{\omega^2} & -iC_{44}\frac{k}{2\alpha_l}\frac{k^2+\alpha_t^2}{\omega^2} & -iC'_{44}\frac{k\alpha'_t}{\omega^2} & iC'_{44}\frac{k}{2\alpha'_l}\frac{k^2+\alpha_t'^2}{\omega^2} \\ -\alpha_t/2\omega^2 & k^2/2\alpha_l\omega^2 & \alpha'_t/2\omega^2 & -k^2/2\alpha'_l\omega^2 \\ \frac{ik}{2\omega^2}\,\mathrm{sgn}x'_3 & -\frac{ik}{2\omega^2}\,\mathrm{sgn}x'_3 & -\frac{ik}{2\omega^2}\,\mathrm{sgn}x'_3 & \frac{ik}{2\omega^2}\,\mathrm{sgn}x'_3 \end{bmatrix}. \tag{2.16}$$

Assigning the lines and columns 1 to 4 of matrices $H$ and $K$ to the indices $t$, $l$, $t'$, and $l'$, respectively, we obtain from Eqs. (2.14)–(2.16)

$$A_i = \frac{1}{\det(\vec{H})}\sum_{j=t,\,l,\,t',\,l'}\det(\vec{A}_{ij})e^{-\alpha_j|x'_3|}, \tag{2.17}$$

where $\vec{A}_{ij}$ is a matrix obtained by replacing column $i$ in $\vec{H}$ by column $j$ of $\vec{K}$.

Finally with the help of Eqs. (2.12), (2.13), and (2.17) we obtain for $x_3>0$

$$g_{xx}(k,\omega\,|x_3,x_3') - g^0_{xx}(k,\omega\,|x_3,x_3') = \frac{1}{\det(\vec{H})}\sum_{i=t,\,l}\sum_{j=t,\,l,\,t',\,l'}\det(\vec{A}_{ij})\,e^{-(\alpha_i|x_3|+\alpha_j|x'_3|)}, \tag{2.18}$$

$$g_{zx}(k,\omega\,|x_3,x_3') - g^0_{zx}(k,\omega\,|x_3,x_3') = \frac{1}{\det(\vec{H})}\sum_{j=t,\,l,\,t',\,l'}\left(\frac{ik}{\alpha_t}\det(\vec{A}_{tj})e^{-\alpha_t|x_3|} + \frac{i\alpha_l}{k}\det(\vec{A}_{lj})e^{-\alpha_l|x_3|}\right)e^{-\alpha_j|x'_3|}. \tag{2.19}$$

For $x_3<0$, the expressions for the Green's functions are obtained by interchanging in Eqs. (2.18) and (2.19) the parameters of the two crystals 1 and 2 and by changing the sign in the second member of (2.19).

In the same manner as described above, one obtains for $x_3>0$, for instance,

$$g_{zz}(k,\omega\,|x_3,x_3') - g^0_{zz}(k,\omega\,|x_3,x_3') = \frac{1}{\det(\tilde{\tilde{H}}')} \sum_{i=t,l} \sum_{j=t,l,t',l'} \det(\tilde{\tilde{A}}'_{ij}) e^{-(\alpha_i|x_3| + \alpha_j|x_3'|)}, \tag{2.20}$$

with

$$g^0_{zz}(k,\omega\,|x_3,x_3') = -\frac{k^2}{2\alpha_t\omega^2}\left(e^{-\alpha_t|x_3-x_3'|} - \frac{\alpha_t\alpha_l}{k^2}\, e^{-\alpha_l|x_3-x_3'|}\right),$$

$$g_{xz}(k,\omega\,|x_3,x_3') - g^0_{xz}(k,\omega\,|x_3,x_3') = -\frac{1}{\det(\tilde{\tilde{H}}')} \sum_{j=t,l,t',l'} \left(\frac{i\alpha_t}{k}\det(\tilde{\tilde{A}}'_{tj})e^{-\alpha_t|x_3|} + \frac{ik}{\alpha_l}\det(\tilde{\tilde{A}}'_{lj})e^{-\alpha_l|x_3|}\right)e^{-\alpha_j|x_3'|},$$

where

$$g^0_{xz}(k,\omega x_3,x_3') = (ik/2\omega^2)\,\mathrm{sgn}(x_3-x_3')(e^{-\alpha_t|x_3-x_3'|} - e^{-\alpha_l|x_3-x_3'|}),$$

$$\tilde{\tilde{H}}' = \begin{bmatrix} iC_{44}(k^2+\alpha_t^2)/k & 2ikC_{44} & -iC'_{44}(k^2+\alpha_t'^2)/k & -2iC'_{44}k \\ -2C_{44}\alpha_t & -C_{44}(k^2+\alpha_t^2)/\alpha_l & -2C'_{44}\alpha'_t & -C'_{44}(k^2+\alpha_t'^2)/\alpha'_l \\ -i\alpha_t/k & -ik/\alpha_l & -i\alpha'_t/k & -ik/\alpha'_l \\ 1 & 1 & -1 & -1 \end{bmatrix},$$

and the matrices $\tilde{\tilde{A}}'_{ij}$ are obtained by replacing column $i$ in $\tilde{\tilde{H}}'$ by column $j$ of $\tilde{\tilde{K}}'$,

$$\tilde{\tilde{K}}' = \begin{bmatrix} iC_{44}\dfrac{k}{2\alpha_t}\dfrac{k^2+\alpha_t^2}{\omega^2} & -iC_{44}\dfrac{k\alpha_l}{\omega^2} & -iC'_{44}\dfrac{k}{2\alpha'_t}\dfrac{k^2+\alpha_t'^2}{\omega^2} & iC'_{44}\dfrac{k\alpha'_l}{\omega^2} \\ C_{44}\dfrac{k^2}{\omega^2}\,\mathrm{sgn}\,x_3' & -C_{44}\dfrac{k^2+\alpha_t^2}{2\omega^2}\,\mathrm{sgn}\,x_3' & -C'_{44}\dfrac{k^2}{\omega^2}\,\mathrm{sgn}\,x_3' & C'_{44}\dfrac{k^2+\alpha_t'^2}{2\omega^2}\,\mathrm{sgn}\,x_3' \\ \dfrac{ik}{2\omega^2}\,\mathrm{sgn}\,x_3' & -\dfrac{ik}{2\omega^2}\,\mathrm{sgn}\,x_3' & -\dfrac{ik}{2\omega^2}\,\mathrm{sgn}\,x_3' & \dfrac{ik}{2\omega^2}\,\mathrm{sgn}\,x_3' \\ k^2/2\alpha_t\omega^2 & -\alpha_l/2\omega^2 & -k^2/2\alpha'_t\omega^2 & \alpha'_l/2\omega^2 \end{bmatrix}.$$

Finally $g_{yy}$ can be written, for $x_3>0$, for example, as

$$g_{yy}(\vec{k},\omega\,|x_3,x_3') - g^0_{yy}(k,\omega\,|x_3,x_3') = [e^{-\alpha_t|x_3|}/2(\alpha_t C_{44}+\alpha'_t C'_{44})] \times\{\rho e^{-\alpha_t|x_3'|}[(\alpha'_t/\alpha_t)C'_{44}/C_{44} - \mathrm{sgn}\,x_3'] + \rho' e^{-\alpha'_t|x_3'|}(\mathrm{sgn}\,x_3' - 1)\}, \tag{2.21}$$

where

$$g^0_{yy}(k\omega\,|\,x_3,x_3') = -(1/2\alpha_t C_t^2)e^{-\alpha_t|x_3-x_3'|}.$$

In Sec. III, we use these Green's functions for the calculation of the mean-square displacements of atoms near an interface.

## III. INTERFACE-ATOM MEAN-SQUARE DISPLACEMENTS

At high temperatures, the atom MSD are given by[5,6]

$$\langle u_\alpha^2(\vec{x})\rangle = -(k_B T/\rho)U_{\alpha\alpha}(\vec{x},\vec{x};0), \tag{3.1}$$

where $T$ is the absolute temperature and $k_B$ is the Boltzmann constant. The Green's function $U_{\alpha\alpha}(\vec{x},\vec{x};0)$ can be obtained[5] from the $g_{\alpha\alpha}(k,0\,|x_3,x_3)$:

$$U_{zz}(\vec{x},\vec{x};0) = \frac{1}{(2\pi)^2}\int_0^{k_c} 2\pi k\,dk\, g_{zz}(k,0\,|x_3,x_3), \tag{3.2a}$$

$$U_{xx}(\vec{x},\vec{x};0) = \frac{1}{(2\pi)^2}\int_0^{2\pi} d\varphi \int_0^{k_c} k\,dk \times[\cos^2\varphi g_{xx}(k,0\,|x_3,x_3) + \sin^2\varphi g_{yy}(k,0\,|x_3,x_3)], \tag{3.2b}$$

$$U_{yy}(\vec{x},\vec{x};0) = \frac{1}{(2\pi)^2}\int_0^{2\pi} d\varphi \int_0^{k_c} k\,dk \times[\sin^2\varphi g_{xx}(k,0\,|x_3,x_3) + \cos^2\varphi g_{yy}(k,0\,|x_3,x_3)], \tag{3.2c}$$

where $k_c$ is a cutoff one has to introduce in order to calculate the MSD of a certain volume of elastic matter. Such a cutoff arises naturally in a lattice theory, where the allowed values of the wave vector are restricted to the first Brillouin zone. The order of magnitude of $k_c$ is the reciprocal of a

lattice spacing. The need to introduce a cutoff arises in the continuum theory because the MSD of a point in an elastic medium is infinite, and one must therefore consider a finite volume. The relationship between this finite volume and the cutoff on the wave vector is the following. We know that in a lattice theory the volume of the first Brillouin zone is proportional to the reciprocal of the volume of a unit cell, or for a crystal with one atom per unit cell, the volume associated with an atom. When we apply a cutoff only to the two components of wave vector parallel to the surface, we are in effect taking a Brillouin zone in the shape of a cylinder whose height is infinite, because there is no restriction on the third component of wave vector. Therefore, the corresponding volume of an atom is represented in real space by a plate whose lateral dimensions are on the order of a lattice spacing, but which is infinitely thin. This partially resolves the problem, but is not entirely satisfactory, because we still do not have a nonzero volume associated with an atom. Later in the paper we introduce a cutoff on the wave-vector component perpendicular to the interface and consider a Debye sphere rather than the cylinder of infinite height. The radius of the Debye sphere can be taken to be $(2\pi/a)(3/4\pi)^{1/3} \cong 3.89/a$, where $a$ is the lattice parameter. The corresponding volume in real space is of order $a^3$ and is therefore nonzero and characteristic of the volume one associates with an atom.

Let us remark that Eqs. (3.2b) and (3.2c) can also be written

$$U_{xx}(\vec{x},\vec{x};0) = U_{yy}(\vec{x},\vec{x};0) = \frac{1}{(2\pi)^2}\int_0^{k_c} 2\pi k\, dk \tfrac{1}{2}[g_{xx}(k,0|x_3,x_3) + g_{yy}(k,0|x_3,x_3)]. \tag{3.2d}$$

In these expressions one takes the value of $g_{\alpha\alpha}$ for $\omega = 0$. We will make an expansion of the $g_{xx}(k,\omega|x_3,x_3)$ for $\omega/c_t k \ll 1$ before taking the limit $\omega = 0$, because otherwise $g_{xx}$ and $g_{zz}$ would have an indeterminant form. Let us introduce

$$\nu = \frac{C_t^2}{C_l^2}, \quad \nu' = \frac{C_t'^2}{C_l'^2}, \quad \gamma = \frac{C_{44}'}{C_{44}}, \quad \phi = kx_3. \tag{3.3}$$

We obtain, for $x_3 > 0$, for example, the following results:

$$g_{\alpha\alpha}(k,0|x_3,x_3) = (1/4kC_t^2)\,[-(1+\nu) + e^{-2kx_3}(\mathcal{E}_\alpha(\phi)/\Delta)], \quad (\alpha = x,z) \tag{3.4a}$$

$$g_{yy}(k,0|x_3,x_3) = (1/2kC_t^2)[-1 + e^{-2kx_3}(\gamma-1)/(\gamma+1)], \tag{3.4b}$$

where

$$\Delta + \gamma^2(1-\nu')(1+\nu) + 2\gamma(1+\nu\nu') + (1+\nu')(1-\nu), \tag{3.5a}$$

$$\mathcal{E}_\alpha(\phi) = \gamma^2(1-\nu')(P_{0\alpha}+P_{1\alpha}\phi+P_{2\alpha}\phi^2) + \gamma\nu'(Q_{0\alpha}+Q_{1\alpha}\phi+Q_{2\alpha}\phi^2) + (1+\nu')(R_{0\alpha}+R_{1\alpha}\phi+R_{2\alpha}\phi^2) \tag{3.5b}$$

and

$$\begin{aligned} &P_{0x} = P_{0z} = (1+\nu)^2; \quad P_{1x} = -P_{1z} = -2(1-\nu^2); \\ &P_{2x} = P_{2z} = 2(1-\nu)^2; \\ &Q_{0x} = Q_{0z} = 2\nu(1+\nu); \quad Q_{1x} = -Q_{1z} = -4(1-\nu^2); \\ &Q_{2x} = Q_{2z} = 4(1-\nu)^2; \\ &R_{0x} = R_{0z} = -(1+\nu^2); \quad R_{1x} = -R_{1z} = 2(1-\nu^2); \\ &R_{2x} = R_{2z} = -2(1-\nu)^2. \end{aligned} \tag{3.5c}$$

In the expressions (3.4) for the $g$, the first term comes from the bulk $g^0_{\alpha\alpha}$ and the second one is the interface contribution. Let us introduce

$$I_n = \int_0^{k_c x_3} X^n e^{-2X}\, dX \quad (n = 0,1,2). \tag{3.6}$$

With these notations and the help of Eqs. (3.1)–(3.6), one obtains in medium 1:

$$\langle u_z^2(x_3)\rangle = \frac{k_B T}{8\pi C_{44}}\left((1+\nu)k_c - \frac{\Delta_z}{\Delta}\frac{1}{x_3}\right), \tag{3.7a}$$

$$\langle u_x^2(x_3)\rangle = \langle u_y^2(x_3)\rangle = \frac{k_B T}{16\pi C_{44}}\left[(3+\nu)k_c - \left(\frac{\Delta x}{\Delta} + \frac{\gamma-1}{\gamma+1}(1-e^{2k_c x_3})\right)\frac{1}{x_3}\right], \tag{3.7b}$$

where the $\Delta_\alpha (\alpha = z \text{ or } x)$ are obtained by replacing $\phi^n$ in $\mathcal{E}_\alpha(\phi)$ by $I_n$. The first terms of these MSD independent of $x_3$ are the bulk values of the MSD of an elastic plate. The second term, which goes to zero when $x_3 \to \infty$, is the interface contribution $\langle u_\alpha^2(x_3)\rangle_I$. Let us remark that in the limit of $C_{44}' \to 0$, the expressions (3.7) are the same as those given by Wallis *et al.*[5] for a semi-infinite crystal.

If we now turn our attention to the bulk contributions, we are immediately faced with the situation that the two bulk components are not equal. The anisotropy is related to the introduction of a Debye cutoff to the two-dimensional wave vector. As has been mentioned, one is dealing with a cylinder of infinite height in wave-vector space and with a plate in real space. One can restore the bulk isotropy by introducing an integration over a Debye sphere rather than over a cylinder. This was done before for a semi-infinite medium.[5] The symmetrized and unsymmetrized results for the surface contributions were almost the same except

in the close neighborhood of the surface ($k_c x_3 \lesssim 1$). In this region, the symmetrized results are more reasonable by comparison with other calculations.[10,11]

We give in the Appendix the symmetrized results. Let us remark that these symmetrized results for the MSD are not continuous across the interface ($\langle u_\alpha^2(+0)\rangle \neq \langle u_\alpha^2(-0)\rangle$). This is easily understood, since for $x_3 = +0$, we calculate the MSD of a sphere of medium 1, and for $x_3 = -0$, the MSD of a sphere of medium 2. In fact for $x_3 = 0$, one has half of these spheres in medium 1 and half in medium 2. With the unsymmetrized results, one is calculating the MSD of a thin plate of matter; the MSD is continuous across the interface under the assumption one is choosing the same cutoff, $k_c$, for both media. However the cutoff $k_c$ is related to the interatomic distance and can be chosen differently for the two media. In an atomic model one would calculate the MSD of atoms located, respectively, at $\pm\frac{1}{2}d$, where $d$ would be the distance between the two surfaces when they are in epitaxy. In general, one may have diffusion of atoms of medium 1 into medium 2 and vice versa. In this more realistic case, it would be even more difficult to define the MSD of atoms in the vicinity of the interface. One sees then, that the only unambiguous term given by elasticity theory is the $1/x_3$ term, which was found[5,6] to be accurate already within a few percent for the second atomic plane below a free surface.

Coming back to Eq. (3.7), and noticing that when $k_c x_3 \gg 1$, $I_0$, $I_1$, and $I_2$ become, respectively, 0.5, 0.25, and 0.25, one has

$$\langle u_\alpha^2(x_3)\rangle_I \simeq (k_B T/16\pi C_{44})(\Gamma_\alpha/x_3), \tag{3.8}$$

where

$$\Gamma_z = (1/\Delta)[-\gamma^2(1-\nu')(\nu^2+3) - 2\gamma\nu'(\nu^2-\nu+2) + (1+\nu')(\nu^2-2\nu+3)], \tag{3.9a}$$

$$\Gamma_x = \Gamma_y = (1/2\Delta)[-\gamma^2(1-\nu')(3\nu^2+1) - 2\gamma\nu'\nu(3\nu-1) + (1+\nu')(3\nu^2-2\nu+1)] + (1-\gamma)/(1+\gamma). \tag{3.9b}$$

This result is the only one which is exact in elasticity theory as it is independent of $k_c$. In the close neighborhood of the interface, the integrals $I_n$ have terms like $e^{-2k_c x_3}$ which have an atomic character and cannot be considered as giving exact results within elasticity theory. They are, however, necessary to obtain a finite value for $\langle u_\alpha^2(0)\rangle_I$.

Let us now specify the coefficients $\Gamma_\alpha$ appearing in the $1/x_3$ laws. For example in the numerator and denominator of $\Gamma_z$ one has polynomials of degree two in $\gamma$ with coefficients depending on $\nu$ and $\nu'$. Let us recall that from the stability of the crystals $\gamma > 0$, and $0 < \nu, \nu' < 0.75$. One finds easily that $\Delta > 0$. The equation $\Gamma_z = 0$ has a negative unacceptable root in $\gamma$ and another positive one we call $\gamma_0 = R(\nu, \nu')$. In the same manner one obtains for medium 2 a positive root $\gamma_0' = [R(\nu', \nu)]^{-1}$ of the equation $\Gamma_z' = 0$.

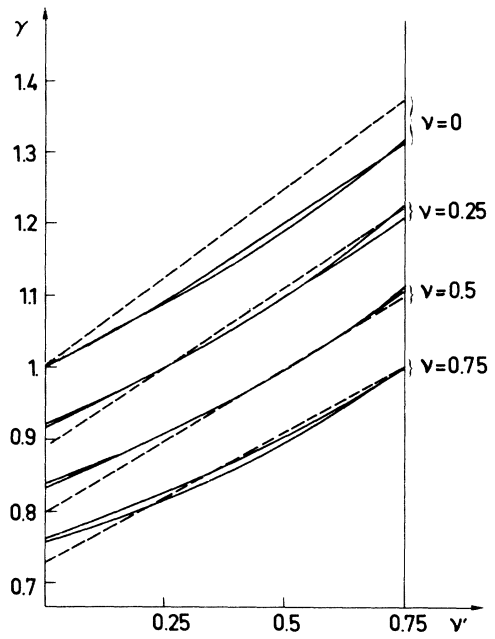


FIG. 1. Determination of the signs of $\Gamma_z$ and $\Gamma_z'$. The curves in full lines give $\Gamma_z = 0$ and $\Gamma_z' = 0$. For given values of $\nu$ and $\nu'$, $\Gamma_z$ and $\Gamma_z'$ are of the same sign if $\gamma$ is between the two full curves and of opposite signs otherwise. Along the broken curve the bulk atom MSD are the same in both media.

Depending on the respective values of $\gamma$, $\gamma_0$, and $\gamma_0'$, the coefficients $\Gamma_z$ and $\Gamma_z'$ can be both positive, both negative, or of opposite signs. Figure 1 shows in the plane $(\nu', \gamma)$ and for a few values of $\nu$, the curves $\Gamma_z = 0$ and $\Gamma_z' = 0$ (full curves); for given values of $\nu$ and $\nu'$, $\Gamma_z$ and $\Gamma_z'$ are of the same sign if $\gamma$ is between the two full curves, and of opposite signs otherwise. In Fig. 1, we have also shown the line $\gamma = (2+\nu')/(2+\nu)$ (broken curve), i.e., the curve corresponding to $\langle u^2\rangle_B = \langle u^2\rangle_{B'}$ when one chooses the same $k_c$ for both media. In a region outside the full curves but between one of them and the broken curve we have $\langle u^2\rangle_B < \langle u^2\rangle_{B'}$ while $\Gamma_z' > 0$, $\Gamma_z < 0$, or vice-versa. Let us remark that for each value of $\nu$ the three curves intersect each other at $\nu' = \nu$ and $\gamma = 1$.

This behavior is different from that obtained for the surface MSD. In that case $\Gamma_z = (\nu^2 - 2\nu + 3)/(1-\nu) > 0$. Starting from the bulk, the MSD always

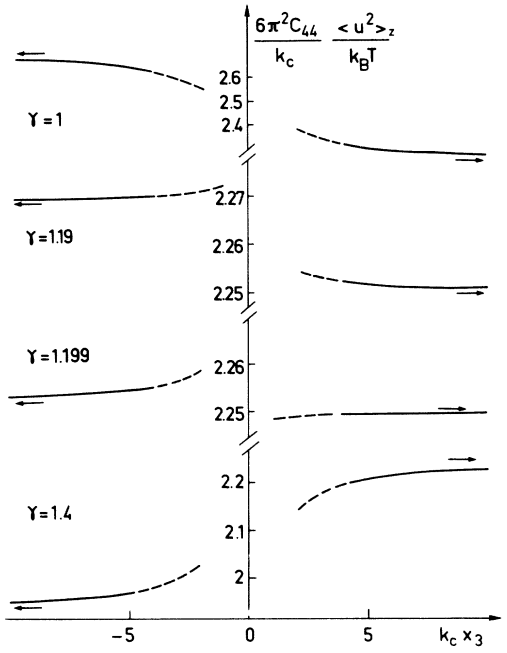


FIG. 2. Different behavior of the atom MSD in the vicinity of the interface for $\nu = 0.25$ and $\nu' = 0.7$. The arrows give the bulk values.

increases when one goes towards a free surface. For an interface, one may have a different and more interesting behavior, illustrated by Fig. 2. In this figure we have represented for $\nu = 0.25$, $\nu' = 0.7$, and for four values of $\gamma$, say $\gamma = 1.1$, 1.19, 1.199, and 1.4, the $x_3^{-1}$ behavior of MSD in each medium (the arrows indicate the bulk MSD).

Finally this discussion is also valid for the MSD parallel to the interface. As a matter of fact the numerator of $\Gamma_x$ is a polynomial $P(\gamma)$, of degree three in $\gamma$, having the following properties: $P(0) > 0$, $dP/d\gamma(\gamma = 0) > 0$, and $dP/d\gamma$ has only one positive root. $P(\gamma)$ has then only one positive root $\tilde{\gamma}_0 = R(\nu, \nu')$. This case is described in Fig. 3 in the same way as in Fig. 1.

We can also compare in one of the two media, for example in medium 1, the coefficients $\Gamma_z$ and $\Gamma_x$. More precisely, one can write

$$\Gamma_x - \Gamma_z = Q(\gamma)/2(1+\gamma)\Delta ,$$

where $Q(\gamma)$ is a polynomial of degree 3 in $\gamma$, with $Q(0) < 0$ and $Q(+\infty) = +\infty$. Therefore $Q(\gamma)$ has at least one positive root. In other words, depending on the values of $\gamma, \nu, \nu'$, one can have $\Gamma_z > \Gamma_x$ or $\Gamma_x > \Gamma_z$. Figure 4 shows in the plane $(\nu', \gamma)$ and for a few values of $\nu$, the curves $\Gamma_z = \Gamma_x$. For given $\nu$ and $\nu'$, we have $\Gamma_z > \Gamma_x$ if $\gamma$ is below this curve and $\Gamma_z < \Gamma_x$ if $\gamma$ is above it. This behavior is also different from that obtained for a semi-infinite crystal where one has always[5] $\Gamma_z > \Gamma_x$.

Let us finally look into the limit of a plane defect which can be defined in an atomic model by supposing for example that one has different interatomic interactions between two adjacent planes. In the above result, if one supposes the two media identical ($\gamma = 1, \nu = \nu'$), Eqs. (3.7) and (3.8) give $\langle u_\alpha^2(x_3)\rangle_I = 0$. One has the results of an infinite

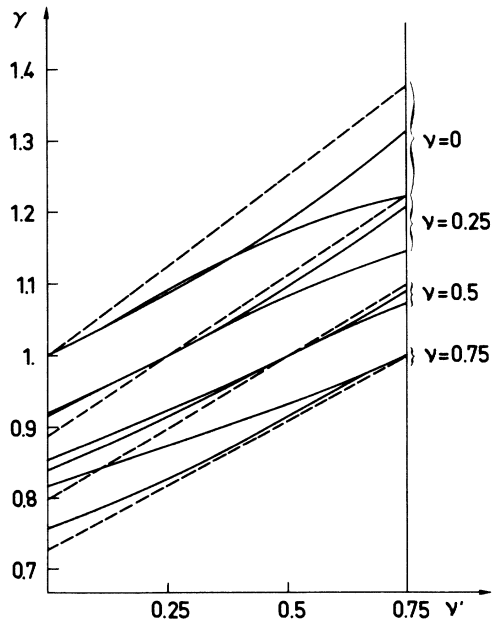


FIG. 3. Determination of the signs of $\Gamma_x$ and $\Gamma_x'$ as in Fig. 1.

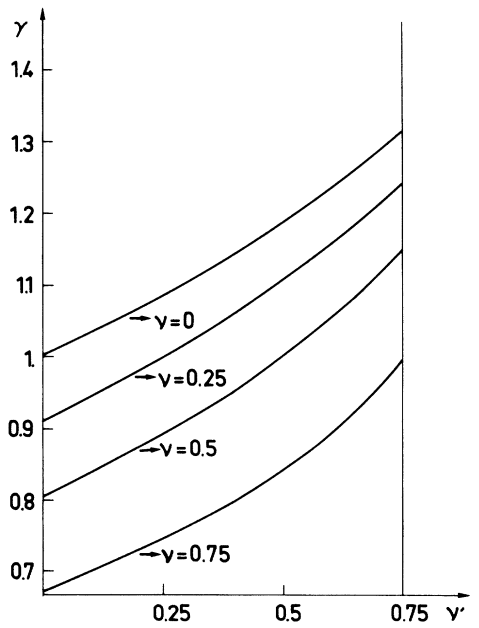


FIG. 4. Determination of the sign of $\Gamma_z - \Gamma_x$. For each value of $\nu$, one has $\Gamma_z > \Gamma_x$ below the curve.

crystal. However in a Montroll-Potts[12] type model, one finds[13] that near a plane defect, the MSD reach their bulk values according to an $x_3^{-2}$ law, rather than $x_3^{-1}$. Such differences near an interface or a plane defect, were also obtained for other physical entities. For example the low-temperature specific heat of an interface[8] goes like $T^2$, while for a plane defect one has[14] a $T^3$ law. One also has similar results for the interaction of an isotopic impurity with an interface,[15] as well as for the interface low-temperature specific heat or the interface magnetization for two coupled Heisenberg ferromagnets.

## IV. CONCLUSION

We have calculated the Green's functions of two isotropic elastic media bounded by a planar interface. The knowledge of these Green's functions enables one to obtain numerous physical properties of an interface.

The Stoneley waves[16] and their existence conditions[17] can be obtained from the poles of these Green's functions, or in other words from the roots of $\det(\tilde{H}) = (\alpha_t \alpha_t' / \alpha_l \alpha_l') \det(\tilde{H}') = 0$ [see Eqs. (2.18)–(2.21)]. We recently generalized this study to the case of an interface between two different hexagonal crystals.[18] The interface Green's functions enabled us also to calculate the interface specific heat at low temperatures.[8] They also enable one to study the scattering of phonons by the interface and by interface defects.

In the present paper, we calculated for the first time the mean-square displacements (MSD) of particles near an interface. The elasticity theory enables one to obtain exactly the $\Gamma_\alpha / x_3$ law ($\alpha = x$, $y$, or $z$) which gives the difference between the interface and the bulk mean-square displacements, a few atomic layers away from the interface. We derived in closed form the coefficients $\Gamma_\alpha$ and $\Gamma'_\alpha$, respectively, for media 1 and 2 and found that they can be either both positive, both negative, or of opposite signs. On the other hand, the coefficients $\Gamma_x = \Gamma_y$, and $\Gamma_z$ of one of the media can satisfy $\Gamma_x > \Gamma_z$ or $\Gamma_z > \Gamma_x$ depending on the respective values of the elastic constants of the two media.

These results are different from those obtained for a free surface[5,7] of an isotropic elastic medium where $\Gamma_\alpha > 0$ (the MSD always increases when one approaches the surface) and $\Gamma_z > \Gamma_x$ (the MSD perpendicular to the surface is always larger than the parallel one).

Finally we have discussed for a few elastic properties the difference between an interface and a bulk plane defect.

## APPENDIX

We give in this Appendix the symmetrized results for the bulk and the interface MSD.

The terms $e^{-\alpha_i |x_3 - x_3'|}$ ($i = t$ or $l$) appearing in the bulk Green's functions can be Fourier analyzed[5] along the direction

$$e^{-\alpha_i |x_3 - x_3'|} = \int_{-\infty}^{+\infty} \frac{dk_z}{2\pi} e^{ik_z |x_3 - x_3'|} \frac{2\alpha_i}{\alpha_i^2 + k_z^2} .$$

In the calculation [Eqs. (3.1) and (3.2)] of the bulk MSD, the Fourier transformation will now be done in the three-dimensional wave vector space $(\vec{k}, k_z)$. Integrating over a sphere of radius $k_c$, one obtains[5]:

$$\langle u_\alpha^2 \rangle_B = \frac{k_B T}{6\pi^2 C_{44}} (2 + \nu) k_c , \quad (\alpha = x, y, z) .$$

In order to use this procedure for the calculation of the interface MSD one does the Fourier transformation of $g_{\alpha\beta}(k, \omega \mid x_3, x_3)$, with the help of the following additional identities:

$$x_3 e^{-2kx_3} = -\int_{-\infty}^{+\infty} \frac{dk_z}{2\pi} e^{2ik_z x_3} \times \left( \frac{1}{k^2 + k_z^2} - \frac{2k^2}{(k^2 + k_z^2)^2} \right) ,$$

$$x_3^2 e^{-2kx_3} = -k \int_{-\infty}^{+\infty} \frac{dk_z}{2\pi} e^{2ik_z x_3} \times \left( \frac{3}{(k^2 + k_z^2)^2} - \frac{4k^2}{(k^2 + k_z^2)^3} \right) ,$$

where we choose $x_3 > 0$, for example, and suppose $k > 0$. Once this Fourier transformation and the integration over a sphere of radius $k_c$ are done, one obtains for the difference between the interface and the bulk MSD

$$\langle u_z^2(x_3) \rangle_I = -\frac{k_B T}{8\pi C_{44}} \frac{\tilde{\Delta}_z}{\Delta} \frac{1}{x_3} , \quad \langle u_x^2(x_3) \rangle_I = \langle u_y^2(x_3) \rangle_I = -\frac{k_B T}{16\pi C_{44}} \left( \frac{\tilde{\Delta}_x}{\Delta} + \frac{2}{\pi} \frac{\gamma - 1}{\gamma + 1} \mathrm{Si}(2\phi_c) \right) \frac{1}{x_3} ,$$

where $\phi_c = k_c x_3$, and the $\tilde{\Delta}_\alpha$ ($\alpha = z$ or $x$) are the expressions one obtains by replacing in $\mathcal{E}_\alpha$ [Eq. (3.5b)] the variables $\phi^0 (\equiv 1)$, $\phi$, and $\phi^2$, respectively, by the quantities $\mathcal{J}_0$, $\mathcal{J}_1$, and $\mathcal{J}_2$ with

$$\mathcal{J}_0 = (1/\pi) \mathrm{Si}(2\phi_c) ,$$

$$\mathcal{J}_1 = 1/2\pi \left[ \cos 2\phi_c / \phi_c - \sin 2\phi_c / 2\phi_c^2 + \mathrm{Si}(2\phi_c) \right] ,$$

$$\mathcal{J}_2 = 1/2\pi \left[ (3/\phi_c^2 + \tfrac{1}{2}) \cos 2\phi_c / \phi_c + (\tfrac{7}{4} - 3/2\phi_c^2) \sin 2\phi_c / \phi_c^2 + \mathrm{Si}(2\phi_c) \right] .$$

In these expressions $\mathrm{Si}(x)$ is the sine integral function.

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†Work supported in part by the U. S. Office of Naval Research under Contract No. N00014-76-C-0121.

[1]See, for example, G. A. Somarjai, *The Principles of Surface Chemistry* (Prentice-Hall, Englewood Cliffs, N. J., 1972), p. 97.

[2]See, for example, R. F. Wallis, Prog. Surf. Sci. 4, 233 (1973).

[3]H. Hainkes, H. Nahr, H. Wilsch, Surf. Sci. 33, 516 (1972); J. R. Bledsoe, S. S. Fisher, *ibid.* 46, 129 (1974); B. Wood, B. F. Mason, B. R. Williams, J. Chem. Phys. 61, 1435 (1974).

[4]J. W. Burton and R. P. Godwin, Phys. Rev. 158, 218 (1967).

[5]R. F. Wallis, A. A. Maradudin, and L. Dobrzynski (unpublished).

[6]L. Dobrzynski and J. Lajzerowicz, Phys. Rev. B 12, 1358 (1975).

[7]J. Lajzerowicz and L. Dobrzynski, Phys. Rev. B 14, 2695 (1976).

[8]B. Djafari-Rouhani and L. Dobrzynski, Phys. Rev. B 14, 2296 (1976).

[9]A. A. Maradudin and D. L. Mills, Ann. Phys. (N.Y.) (to be published); see also L. Dobrzynski and A. A. Maradudin, Phys. Rev. B 14, 2200 (1976).

[10]A. A. Maradudin and J. Melngailis, Phys. Rev. 133 A1188 (1964).

[11]R. L. Dennis and D. L. Huber, Phys. Rev. B 5, 4717 (1972).

[12]E. W. Montroll and R. B. Potts, Phys. Rev. 100, 525 (1955).

[13]B. Djafari-Rouhani and L. Dobrzynski (unpublished).

[14]B. Djafari-Rouhani, P. Masri, L. Dobrzynski, Phys. Rev. B (to be published).

[15]The interaction free energy of an isotopic impurity with a free surface decreases like $x_3^{-4}$ where $x_3$ is the distance to the surface; see A. A. Maradudin, E. W. Montroll, G. H. Weiss, and I. P. Ipatova, Solid State Phys. Suppl. 3, 620 (1971). One has still a $x_3^{-4}$ law for an interface, but a $x_3^{-5}$ law for a plane defect (Ref. 13).

[16]R. Stoneley, Proc. R. Soc. A 106, 421 (1927).

[17]J. C. Scholte, Proc. Acad. Sci. Amst. 45, 20 (1942); 45, 159 (1942).

[18]B. Djafari-Rouhani and L. Dobrzynski, Surf. Sci. (to be published).