Elastic interaction and self-relaxation energies of coherently strained conical islands

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Projection force density methods, based on the surface Green's function approach, are employed to obtain analytical expressions for the elastic interaction and self-relaxation energies of coherently strained conical islands. These results are used to evaluate the island chemical potential as the basis for coarsening models and a stability analysis of elastically interacting quantum dot arrays.

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I. INTRODUCTION

The formation of coherently strained islands on surfaces during thin film deposition is an attractive means of fabricating nanostructure arrays for possible applications in novel quantum dot devices.[1] However, for many applications, island size uniformity is critical. It is therefore of central importance to understand the key factors influencing the stability and dynamical evolution of arrays during coarsening.[2–15] In this regard, it is known that elastic interactions between islands can significantly influence the coarsening kinetics and thermodynamic stability of quantum dot arrays.[10–13,15]

In this paper, we present a detailed derivation of analytical expressions for the elastic self-relaxation and interaction energy between surface islands of a conical shape. These results facilitate the derivation of the island chemical potential which has been used to investigate the dynamics of strained island coalescence[15] and the metastability of ultradense arrays.[13] The present work fully addresses the approximations underlying the basic expressions of the cone model and highlights the techniques employed to derive the results which serves as a template for extension of the analysis to other, nonconical, quantum dot geometries.

II. FORMULATION OF THE PROBLEM

Consider the elastic self-relaxation and interaction energy of a system of three-dimensional (3D) islands which elastically interact via the strained substrate. We assume that the islands and substrate/wetting layer have equal elastic constants and that the tilt angle of the island side facets (or surface) $\vartheta \ll \pi/4$. It is further assumed all materials are elastically isotropic so that we can employ the surface Green's function G_{ij} for an isotropic solid.[16]

In the approximation of shallow islands, it is convenient to describe the shape and the arrangement of the islands by the surface profile function $z=\zeta(\mathbf{r})$, where $\mathbf{r}=(x,y)$ is the two-dimensional (2D) position vector. Then the approximation of shallow islands implies that $|\nabla\zeta| \ll 1$. Thus, the elastic displacement field $u_i(\mathbf{r})$ can be expanded in power series over $\nabla\zeta$. The zero-order term is the displacement field in the approximation of the flat surface. The first-order term is given by[17]

$$u_i^{(1)}(\mathbf{r},z) = \int d^2\mathbf{r}' G_{ij}(\mathbf{r}-\mathbf{r}';z,z')\Big|_{z'=0} \sigma_{j\alpha}^{(0)}[-\nabla_\alpha\zeta(\mathbf{r}')]. \tag{2.1}$$

Here $\sigma_{ij}^{(0)}$ is the stress tensor in the planar heteroepitaxial film, i,j are 3D indices, and α is the 2D index. The first-order correction to the strain energy equals[18]

$$\begin{aligned}\Delta E_{\mathrm{el}}^{(1)} &= \frac{1}{2}\int d^2\mathbf{r} f_i(\mathbf{r}) u_i(\mathbf{r}) \\ &= \frac{1}{2}\int d^2\mathbf{r}\int d^2\mathbf{r}'[-\nabla_\alpha\zeta(\mathbf{r})]\sigma_{\alpha i}^{(0)} \\ &\quad \times G_{ij}(\mathbf{r}-\mathbf{r}';z,z')\Big|_{\substack{z=0\\ z'=0}} \sigma_{j\beta}^{(0)}[-\nabla_\beta\zeta(\mathbf{r}')],\end{aligned} \tag{2.2}$$

where $f_j(\mathbf{r})=\sigma_{j\alpha}^{(0)}[-\nabla_\alpha\zeta(\mathbf{r})]$ is the projected force density at the surface. From this point onward, we will only calculate quantities defined on the surface, i.e., at $z=0$ and will consequently omit the argument z.

In the heteroepitaxial system where both the substrate and the deposited material are cubic semiconductors, the lattice mismatch is isotropic, and the stress tensor in the planar film $\sigma_{\alpha i}^{(0)}$ equals

$$\sigma_{\alpha i}^{(0)} = \frac{Y}{1-\nu}\varepsilon_0\delta_{\alpha i}, \tag{2.3}$$

where Y is the Young's modulus, ν is the Poisson ratio, and ε_0 is the lattice mismatch. The integrand in Eq. (2.2) is nonzero only on the projected side surfaces of the islands. By decomposing each integral in Eq. (2.2) into the sum of the integrals over projected surfaces of individual islands, and by substituting Eq. (2.3) into Eq. (2.2), one obtains the energy as follows:

$$\begin{aligned}\Delta E_{\mathrm{el}} = \sum_i \frac{1}{2}\left(\frac{Y}{1-\nu}\right)^2 \int_{A_i} d^2\mathbf{r}\int_{A_i} d^2\mathbf{r}'[\nabla_\alpha\zeta(\mathbf{r})]G_{\alpha\beta}(\mathbf{r}-\mathbf{r}';0,0) \\ \times[\nabla_\beta\zeta(\mathbf{r}')]\end{aligned} \tag{2.4a}$$

$$+\sum_i \sum_{j<i} \left(\frac{Y}{1-\nu}\right)^2 \int_{A_i} d^2\mathbf{r} \int_{A_j} d^2\mathbf{r}' [\nabla_\alpha \zeta(\mathbf{r})] \times G_{\alpha\beta}(\mathbf{r}-\mathbf{r}';0,0)[\nabla_\beta \zeta(\mathbf{r}')]. \quad (2.4b)$$

Every term in the single sum of Eq. (2.4a) is the elastic relaxation energy of a given *i*th island of projected area A_i, whereas every term in the double sum of Eq. (2.4b) is the elastic interaction energy between the *i*th and the *j*th island. The Green's tensor on the surface is given by[16]

$$G_{\alpha\beta}(\mathbf{r}-\mathbf{r}';0,0) = \frac{1+\nu}{\pi Y}\left[\frac{(1-\nu)\delta_{\alpha\beta}}{|\mathbf{r}-\mathbf{r}'|} + \nu\frac{(\mathbf{r}-\mathbf{r}')_\alpha(\mathbf{r}-\mathbf{r}')_\beta}{|\mathbf{r}-\mathbf{r}'|^3}\right]. \quad (2.5)$$

III. ELASTIC INTERACTION ENERGY BETWEEN TWO CONICAL ISLANDS

Consider the interaction energy of two islands, i.e., a single term from the double sum of Eq. (2.4b). By substituting the Green's tensor from Eq. (2.5) into the integrand and integrating by parts, one obtains

$$E_{\text{inter}} = \frac{1+\nu}{1-\nu}\frac{1}{\pi} Y\varepsilon_0^2 \int_{A_i} d^2\mathbf{r}\zeta(\mathbf{r}) \int_{A_j} d^2\mathbf{r}'\zeta(\mathbf{r}')\frac{1}{|\mathbf{r}-\mathbf{r}'|^3}. \quad (3.1)$$

If the distance between the two islands is much larger than the lateral size of the island, one can remove the term $|\mathbf{r}-\mathbf{r}'|^{-3}$ from the integral. The remaining integrals will then give the product of two volumes and

$$E_{\text{inter}} = \frac{1+\nu}{1-\nu}\frac{1}{\pi} Y\varepsilon_0^2 V_1 V_2 \frac{1}{R^3}, \quad (3.2)$$

where R is the distance between the centers of the bases of two islands. This result gives the interaction energy in the dipole-dipole approximation.

It is convenient to introduce the following quantity:

$$W_0 = \frac{Y}{1-\nu}\varepsilon_0^2, \quad (3.3)$$

which is the elastic strain energy density in a flat uniformly strained film. Then, the interaction energy given by Eq. (3.1) reduces to

$$E_{\text{inter}} = \frac{1+\nu}{\pi} W_0 \int_{A_i} d^2\mathbf{r}\zeta(\mathbf{r}) \int_{A_j} d^2\mathbf{r}'\zeta(\mathbf{r}')\frac{1}{|\mathbf{r}-\mathbf{r}'|^3}. \quad (3.4)$$

We note here that, for a dense array of islands, the dipole-dipole approximation is no longer valid, and it is important to know the accurate expression for the interaction energy of two closely spaced islands.

To evaluate the interaction energy of two axially symmetric islands, it is convenient to introduce polar coordinates, r_1, φ_1 for the first island, and r_2, φ_2 for the second island. Then the interaction energy Eq. (3.4) reduces to

$$E_{\text{inter}} = \frac{1+\nu}{\pi} W_0 \int_0^{\rho_1} dr_1 r_1 \zeta(r_1) \int_0^{2\pi} d\varphi_1 \int_0^{\rho_2} dr_2 r_2 \zeta(r_2) \times \int_0^{2\pi} d\varphi_2 \frac{1}{|\mathbf{R}+\mathbf{r}_1-\mathbf{r}_2|^3}. \quad (3.5)$$

Here ρ_1 and ρ_2 are radii of the island bases. If one first integrates over φ_1 and φ_2, this will provide the interaction energies between two rings. Further integration over r_1 and r_2 will give the interaction energy between the two cones.

To evaluate the integral in Eq. (3.5) we employ the useful expression

$$\frac{1}{|\mathbf{r}-\mathbf{r}'|} = \sum_{m=-\infty}^{\infty} \int_0^\infty dk J_m(kr) J_m(kr') \exp[im(\varphi-\varphi')] \quad (3.6)$$

given by Rickman and Srolovitz.[19] Here r and r' are the radii of the two points, φ and φ' are the polar angles of the two points, and J_m is a Bessel function of order m. The derivation of Eq. (3.6) is provided in Appendix B. The integral of Eq. (3.6) can be evaluated[19] using tables of integrals,[20]

$$\frac{1}{|\mathbf{r}-\mathbf{r}'|} = \text{Re}\sum_{m=0}^{\infty} \frac{(2-\delta_{m0})\Gamma\left(m+\frac{1}{2}\right)}{\Gamma(m+1)\Gamma\left(\frac{1}{2}\right)} \exp[im(\varphi-\varphi')]\left(\frac{r_<^m}{r_>^{m+1}}\right) \times {}_2F_1\left(m+\frac{1}{2},\frac{1}{2};m+1;(r_</r_>)^2\right), \quad (3.7)$$

where $r_<$ ($r_>$) is the smaller (larger) of r and r', ${}_2F_1[m+1/2, 1/2; m+1; (r_</r_>)^2]$ is a hypergeometric function, and Re means the real part.

To evaluate the integral of Eq. (3.5), it is useful to consider the expansion of $|\mathbf{r}-\mathbf{r}'|^{-3}$ similar to Eq. (3.7). We note that

$$\frac{1}{|\mathbf{r}-\mathbf{r}'|^3} = \nabla^2 \frac{1}{|\mathbf{r}-\mathbf{r}'|}, \quad (3.8)$$

and write down the Laplacian in polar coordinates

$$\nabla^2 = \frac{1}{r_>}\frac{\partial}{\partial r_>}\left(r_>\frac{\partial}{\partial r_>}\right) + \frac{1}{r_>^2}\frac{\partial^2}{\partial\varphi^2}. \quad (3.9)$$

Expanding the hypergeometric function ${}_2F_1[m+\frac{1}{2},\frac{1}{2};m+1;(r_</r_>)^2]$ in power series over $(r_</r_>)^2$,

$$ {}_2F_1\left(m+\frac{1}{2},\frac{1}{2};m+1;(r_</r_>)^2\right)=\sum_{p=0}^{\infty}\frac{\Gamma\left(m+\frac{1}{2}+p\right)\Gamma\left(\frac{1}{2}+p\right)\Gamma(m+1)}{\Gamma\left(m+\frac{1}{2}\right)\Gamma\left(\frac{1}{2}\right)\Gamma(m+1+p)\Gamma(1+p)}\left(\frac{r_\le}{r_>}\right)^{2p}, \tag{3.10} $$

substituting Eq. (3.10) into Eq. (3.7), and applying the Laplacian from Eq. (3.9), one obtains the following expansion:

$$ \begin{aligned}\frac{1}{|\mathbf{r}-\mathbf{r}'|^3}&=\mathrm{Re}\sum_{m=0}^{\infty}\frac{(2-\delta_{m0})\Gamma\left(m+\frac{1}{2}\right)}{\Gamma(m+1)\Gamma\left(\frac{1}{2}\right)}\exp[im(\varphi-\varphi')]\left(\frac{r_<^m}{r_>^{m+3}}\right)\\&\times\sum_{p=0}^{\infty}\frac{\Gamma\left(m+\frac{1}{2}+p\right)\Gamma\left(\frac{1}{2}+p\right)\Gamma(m+1)}{\Gamma\left(m+\frac{1}{2}\right)\Gamma\left(\frac{1}{2}\right)\Gamma(m+1+p)\Gamma(1+p)}[(2p+m+1)^2-m^2]\left(\frac{r_\le}{r_>}\right)^{2p}\\&=4\mathrm{Re}\sum_{m=0}^{\infty}\frac{(2-\delta_{m0})\Gamma\left(m+\frac{1}{2}\right)}{\Gamma(m+1)\Gamma\left(\frac{1}{2}\right)}\exp[im(\varphi-\varphi')]\left(\frac{r_<^m}{r_>^{m+3}}\right)\\&\times\sum_{p=0}^{\infty}\frac{\Gamma\left(m+\frac{1}{2}+p\right)\Gamma\left(\frac{1}{2}+p\right)\Gamma(m+1)}{\Gamma\left(m+\frac{1}{2}\right)\Gamma\left(\frac{1}{2}\right)\Gamma(m+1+p)\Gamma(1+p)}\left(p+\frac{1}{2}\right)\left(p+\frac{1}{2}+m\right)\left(\frac{r_\le}{r_>}\right)^{2p}\\&=4\mathrm{Re}\sum_{m=0}^{\infty}\frac{(2-\delta_{m0})\Gamma\left(m+\frac{1}{2}\right)}{\Gamma(m+1)\Gamma\left(\frac{1}{2}\right)}\exp[im(\varphi-\varphi')]\left(\frac{r_<^m}{r_>^{m+3}}\right)\sum_{p=0}^{\infty}\frac{\Gamma\left(m+\frac{3}{2}+p\right)\Gamma\left(\frac{3}{2}+p\right)\Gamma(m+1)}{\Gamma\left(m+\frac{1}{2}\right)\Gamma\left(\frac{1}{2}\right)\Gamma(m+1+p)\Gamma(1+p)}\left(\frac{r_\le}{r_>}\right)^{2p}.\end{aligned} \tag{3.11} $$

Now we substitute Eq. (3.11) into the integrand of Eq. (3.5) and integrate over φ_1. In this integration the smaller of the two radii $r_<$ is the radius of the ring r_1, and the larger $r_>$ is the distance between the center of the first ring and the current point on the second ring, i.e., $r_>=|\mathbf{R}-\mathbf{r}_2|$. After the integration over φ_1, only the axially symmetric part (with $m=0$) of the expansion in Eq. (3.11) remains. This integral equals

$$ \begin{aligned}I_1=\int_0^{2\pi}d\varphi_1\frac{1}{|\mathbf{r}-\mathbf{r}'|^3}&=4(2\pi)\frac{\Gamma\left(\frac{1}{2}\right)}{\Gamma(1)\Gamma\left(\frac{1}{2}\right)}\left(\frac{1}{r_>^3}\right)\sum_{p=0}^{\infty}\frac{\Gamma\left(\frac{3}{2}+p\right)\Gamma\left(\frac{3}{2}+p\right)\Gamma(1)}{\Gamma\left(\frac{1}{2}\right)\Gamma\left(\frac{1}{2}\right)\Gamma(1+p)\Gamma(1+p)}\left(\frac{r_1}{r_>}\right)^{2p}\\&=4(2\pi)\sum_{p=0}^{\infty}\left[\frac{\Gamma\left(\frac{3}{2}+p\right)}{\Gamma\left(\frac{1}{2}\right)\Gamma(1+p)}\right]^2\frac{r_1^{2p}}{r_>^{2p+3}}=(2\pi)\sum_{p=0}^{\infty}\left[\frac{\Gamma\left(\frac{3}{2}+p\right)}{\Gamma\left(\frac{3}{2}\right)\Gamma(1+p)}\right]^2\frac{r_1^{2p}}{r_>^{2p+3}}.\end{aligned} \tag{3.12} $$

We note again that $r_>$ in Eq. (3.12) is the distance between the center of the base of the first ring and the current point on the second ring. To perform the second integration over the position of the point on the second ring in Eq. (3.5), i.e., over φ_2, it is necessary to expand $1/r_>^{2p+3}$ in each term of the series in Eq. (3.12) in a way similar to expansions in Eqs. (3.7) and (3.11). To carry out such an expansion, we again note that $r_>=|\mathbf{R}-\mathbf{r}_2|$, where $\mathbf{R}$ is the vector connecting the centers of two disks, and $\mathbf{r}_2$ is the vector connecting the center of the second disk with the current point on the disk. Then using the identity

$$\frac{1}{|\mathbf{R}-\mathbf{r}_2|^{3+2p}} = \frac{1}{3^2\times 5^2\times\cdots(2p+1)^2}(\nabla^2)^{p+1}\frac{1}{|\mathbf{R}-\mathbf{r}_2|^1}$$
$$= \frac{1}{2^{2p}}\left[\frac{1}{\frac{3}{2}\times\frac{5}{2}\times\cdots\left(p+\frac{1}{2}\right)}\right]^2(\nabla^2)^{p+1}\frac{1}{|\mathbf{R}-\mathbf{r}_2|^1}$$
$$= \frac{1}{2^{2p}}\left[\frac{\Gamma\left(\frac{3}{2}\right)}{\Gamma\left(\frac{3}{2}+p\right)}\right]^2(\nabla^2)^{p+1}\frac{1}{|\mathbf{R}-\mathbf{r}_2|^1} = \frac{1}{2^{2p}}\left[\frac{\Gamma\left(\frac{3}{2}\right)}{\Gamma\left(\frac{3}{2}+p\right)}\right]^2(\nabla^2)^p\frac{1}{|\mathbf{R}-\mathbf{r}_2|^3}, \tag{3.13}$$

and substituting the expansion of $|\mathbf{R}-\mathbf{r}_2|^{-3}$ from Eq. (3.11) into Eq. (3.13), we obtain

$$\frac{1}{|\mathbf{R}-\mathbf{r}_2|^{3+2p}} = \frac{1}{2^{2p}}\left[\frac{\Gamma\left(\frac{3}{2}\right)}{\Gamma\left(\frac{3}{2}+p\right)}\right]^2(\nabla^2)^p\left[4\mathrm{Re}\sum_{m=0}^{\infty}\frac{(2-\delta_{m0})\Gamma\left(m+\frac{1}{2}\right)}{\Gamma(m+1)\Gamma\left(\frac{1}{2}\right)}\exp[im(\Phi-\varphi_2)]\right.$$
$$\left.\times\left(\frac{r_2^m}{R^{m+3}}\right)\sum_{q=0}^{\infty}\frac{\Gamma\left(m+\frac{3}{2}+q\right)\Gamma\left(\frac{3}{2}+q\right)\Gamma(m+1)}{\Gamma\left(m+\frac{1}{2}\right)\Gamma\left(\frac{1}{2}\right)\Gamma(m+1+q)\Gamma(1+q)}\left(\frac{r_2}{R}\right)^{2q}\right]. \tag{3.14}$$

Here Φ is the polar angle of the vector $\mathbf{R}$, and φ_2 is the polar angle corresponding to the current point on the ring. Since we aim to integrate over φ_2, we need only axially symmetric terms with $m=0$. Keeping these terms only, we replace the Laplacian by its symmetric part $\nabla^2\to R^{-1}(\partial/\partial R)R(\partial/\partial R)$. Thus, Eq. (3.14) reduces to

$$\frac{1}{|\mathbf{R}-\mathbf{r}_2|^{3+2p}} = \frac{1}{2^{2p}}\left[\frac{\Gamma\left(\frac{3}{2}\right)}{\Gamma\left(\frac{3}{2}+p\right)}\right]^2\left(\frac{1}{R}\frac{d}{dR}R\frac{d}{dR}\right)^p\left[4\sum_{q=0}^{\infty}\left[\frac{\Gamma\left(\frac{3}{2}+q\right)}{\Gamma\left(\frac{1}{2}\right)\Gamma(1+q)}\right]^2\frac{r_2^{2q}}{R^{2q+3}}\right] + \text{terms with } m\neq 0. \tag{3.15}$$

Applying the symmetric part of the Laplacian p times in Eq. (3.15), we obtain

$$\frac{1}{|\mathbf{R}-\mathbf{r}_2|^{3+2p}} = \frac{1}{2^{2p}}\left[\frac{\Gamma\left(\frac{3}{2}\right)}{\Gamma\left(\frac{3}{2}+p\right)}\right]^2\left[4\sum_{q=0}^{\infty}\left[\frac{\Gamma\left(\frac{3}{2}+q\right)}{\Gamma\left(\frac{1}{2}\right)\Gamma(1+q)}\right]^2\left[(2q+3)\cdots(2q+2p+1)\right]^2\frac{r_2^{2q}}{R^{2q+2p+3}}\right] + \text{terms with } m\neq 0,$$
$$= \left[\frac{\Gamma\left(\frac{3}{2}\right)}{\Gamma\left(\frac{3}{2}+p\right)}\right]^2\left[\sum_{q=0}^{\infty}\left[\frac{\Gamma\left(\frac{3}{2}+q\right)}{\Gamma\left(\frac{3}{2}\right)\Gamma(1+q)}\right]^2\left[\left(q+\frac{3}{2}\right)\cdots\left(q+p+\frac{1}{2}\right)\right]^2\frac{r_2^{2q}}{R^{2q+2p+3}}\right] + \text{terms with } m\neq 0,$$
$$= \left[\frac{\Gamma\left(\frac{3}{2}\right)}{\Gamma\left(\frac{3}{2}+p\right)}\right]^2\sum_{q=0}^{\infty}\left[\frac{\Gamma\left(\frac{3}{2}+q\right)}{\Gamma\left(\frac{3}{2}\right)\Gamma(1+q)}\right]^2\left[\frac{\Gamma\left(q+p+\frac{3}{2}\right)}{\Gamma\left(q+\frac{3}{2}\right)}\right]^2\frac{r_2^{2q}}{R^{2q+2p+3}} + \text{terms with } m\neq 0,$$
$$= \left[\frac{\Gamma\left(\frac{3}{2}\right)}{\Gamma\left(\frac{3}{2}+p\right)}\right]^2\sum_{q=0}^{\infty}\left[\frac{\Gamma\left(q+p+\frac{3}{2}\right)}{\Gamma\left(\frac{3}{2}\right)\Gamma(1+q)}\right]^2\frac{r_2^{2q}}{R^{2q+2p+3}} + \text{terms with } m\neq 0. \tag{3.16}$$

Now let us substitute the expansion in Eq. (3.15) into Eq. (3.12) and integrate over φ_2. Then the term with $m=0$ will be multiplied by (2π), and the other terms will vanish. Hence,

$$I_2 = \int_0^{2\pi} d\varphi_2 \int_0^{2\pi} d\varphi_1 \frac{1}{|\mathbf{r}-\mathbf{r}'|^3} = (2\pi)^2 \sum_{p=0}^{\infty}\sum_{q=0}^{\infty} \left[\frac{\Gamma\left(\frac{3}{2}+p\right)}{\Gamma\left(\frac{3}{2}\right)\Gamma(1+p)}\right]^2 \times \left[\frac{\Gamma\left(\frac{3}{2}\right)}{\Gamma\left(\frac{3}{2}+p\right)}\right]^2 \left[\frac{\Gamma\left(q+p+\frac{3}{2}\right)}{\Gamma\left(\frac{1}{2}\right)\Gamma(1+q)}\right]^2 \frac{r_1^{2p} r_2^{2q}}{R^{2q+2p+3}}. \tag{3.17}$$

Further straightforward simplification yields

$$I_2 = (2\pi)^2 \sum_{p=0}^{\infty}\sum_{q=0}^{\infty} \left[\frac{\Gamma\left(\frac{3}{2}+p+q\right)}{\Gamma\left(\frac{3}{2}\right)\Gamma(p+1)\Gamma(q+1)}\right]^2 \frac{r_1^{2p} r_2^{2q}}{R^{2q+2p+3}}. \tag{3.18}$$

It is now convenient to change the order of summation, and to introduce a new variable $s=p+q$. Then the outer summation will be carried out over s, from 0 to ∞, and the inner summation will be carried out over p from 0 to s. Hence,

$$I_2 = (2\pi)^2 \sum_{s=0}^{\infty} \left\{ \sum_{p=0}^{s} \left[\frac{r_1^p r_2^{s-p}}{\Gamma(p+1)\Gamma(s-p+1)}\right]^2 \right\} \times \left[\frac{\Gamma\left(\frac{3}{2}+s\right)}{\Gamma\left(\frac{3}{2}\right)}\right]^2 \frac{1}{R^{3+2s}}. \tag{3.19}$$

The surface profile of the cone is

$$\zeta(r) = \tan\vartheta_{1,2}(\rho_{1,2}-r), \text{ if } \rho_{1,2} > r. \tag{3.20}$$

By substituting Eqs. (3.19) and (3.20) into Eq. (3.5), we obtain the interaction energy

$$E_{\text{inter}} = \frac{1+\nu}{\pi} W_0 (2\pi)^2 (\tan\vartheta_1) \times (\tan\vartheta_2) \sum_{s=0}^{\infty} \left\{ \sum_{p=0}^{s} \left[\frac{1}{\Gamma(p+1)\Gamma(s-p+1)}\right]^2 \times \int_0^{\rho_1} dr_1 (\rho_1 - r_1) r_1^{1+2p} \int_0^{\rho_2} dr_2 (\rho_2 - r_2) r_2^{1+2(s-p)} \right\} \times \left[\frac{\Gamma\left(\frac{3}{2}+s\right)}{\Gamma\left(\frac{3}{2}\right)}\right]^2 \frac{1}{R^{3+2s}}. \tag{3.21}$$

Evaluation of the integrals over r_1 and r_2 yields

$$E_{\text{inter}} = \frac{1+\nu}{\pi} W_0 (2\pi)^2 \frac{\rho_1^3}{6}\frac{\rho_2^3}{6} (\tan\vartheta_1) \times (\tan\vartheta_2) \sum_{s=0}^{\infty} \left\{ \sum_{p=0}^{s} \left[\frac{\rho_1^p \rho_2^{s-p}}{\Gamma(p+1)\Gamma(s-p+1)}\right]^2 \times \frac{\frac{3}{2}}{(p+1)\left(p+\frac{3}{2}\right)} \frac{\frac{3}{2}}{(s-p+1)\left(s-p+\frac{3}{2}\right)} \right\} \times \left[\frac{\Gamma\left(\frac{3}{2}+s\right)}{\Gamma\left(\frac{3}{2}\right)}\right]^2 \frac{1}{R^{3+2s}}. \tag{3.22}$$

It is convenient to express the interaction energy in terms of island volumes. By substituting $\rho_{1,2}=(3\pi^{-1}\cot\vartheta_{1,2}V_{1,2})^{1/3}$ into Eq. (3.22) one obtains the interaction energy in the following form:

$$E_{\text{inter}} = \frac{1+\nu}{\pi} W_0 V_1 V_2 \frac{1}{R^3} F\left(\frac{\rho_1}{R}; \frac{\rho_2}{R}\right). \tag{3.23}$$

Here $F(\eta_1, \eta_2)$ gives the correction factor with respect to the interaction energy of two remote islands [Eq. (3.2)] and is given by

$$F(\eta_1,\eta_2) = \sum_{s=0}^{\infty} \left\{ \left[\frac{\Gamma\left(\frac{3}{2}+s\right)}{\Gamma\left(\frac{3}{2}\right)}\right]^2 \sum_{p=0}^{s} \left[\frac{\eta_1^p \eta_2^{s-p}}{\Gamma(p+1)\Gamma(s-p+1)}\right]^2 \times \frac{\frac{3}{2}}{(p+1)\left(p+\frac{3}{2}\right)} \frac{\frac{3}{2}}{(s-p+1)\left(s-p+\frac{3}{2}\right)} \right\}. \tag{3.24}$$

The correction factor is equal to unity if $\eta_1 \to 0$ and $\eta_2 \to 0$, and E_{inter} approaches the interaction energy obtained in the dipole-dipole approximation.

IV. ELASTIC SELF-RELAXATION ENERGY OF A CONICAL ISLAND

Consider now the elastic relaxation of a single cone, i.e., a single term from the sum in Eq. (2.4a). Inserting Eqs. (2.5) and (3.3) in Eq. (2.4a) gives

$$\Delta E_{\text{self}} = \frac{1}{2\pi}\frac{1+\nu}{1-\nu}W_0 \int d^2\mathbf{r} \int d^2\mathbf{r}' n_\alpha(\mathbf{r}) \left[\frac{(1-\nu)\delta_{\alpha\beta}}{|\mathbf{r}-\mathbf{r}'|} + \nu \frac{(\mathbf{r}-\mathbf{r}')_\alpha (\mathbf{r}-\mathbf{r}')_\beta}{|\mathbf{r}-\mathbf{r}'|^3} \right] n_\beta(\mathbf{r}'), \tag{4.1}$$

where $n_\alpha(\mathbf{r})$ is the surface projection of the normal vector. In the integrand of Eq. (4.1) we make the substitution

$$\frac{(\mathbf{r}-\mathbf{r}')_\alpha (\mathbf{r}-\mathbf{r}')_\beta}{|\mathbf{r}-\mathbf{r}'|^3} = \frac{\delta_{\alpha\beta}}{|\mathbf{r}-\mathbf{r}'|} - \nabla_\alpha \nabla_\beta |\mathbf{r}-\mathbf{r}'|. \tag{4.2}$$

Then, inserting Eq. (4.2) into Eq. (4.1), one obtains the elastic relaxation energy as follows:

$$\Delta E_{\text{self}} = \frac{1}{2\pi}\frac{1+\nu}{1-\nu}W_0 \int d^2\mathbf{r} \int d^2\mathbf{r}' n_\alpha(\mathbf{r}) \times \left[\frac{\delta_{\alpha\beta}}{|\mathbf{r}-\mathbf{r}'|} - \nu \nabla_\alpha \nabla_\beta |\mathbf{r}-\mathbf{r}'| \right] n_\beta(\mathbf{r}'). \tag{4.3}$$

Now, it is convenient to partition the integration over $\mathbf{r}$ and $\mathbf{r}'$ in Eq. (4.3) into an integration over radii and angles. This procedure yields

$$\Delta E_{\text{self}} = \frac{1}{2\pi}\frac{1+\nu}{1-\nu}W_0 \int_0^\rho dr r \int_0^\rho dr' r' J(r,r'), \tag{4.4}$$

where the quantity $J(r,r')$ is proportional to the elastic interaction between *two rings*

$$J(r,r') = \int_0^{2\pi} d\varphi \int_0^{2\pi} d\varphi' n_\alpha(\mathbf{r}) \left[\frac{\delta_{\alpha\beta}}{|\mathbf{r}-\mathbf{r}'|} - \nu \nabla_\alpha \nabla_\beta |\mathbf{r} - \mathbf{r}'| \right] n_\beta(\mathbf{r}'). \tag{4.5}$$

We now Fourier transform all quantities in the integrand of Eq. (4.5) and, afterwards, calculate the integral in $\mathbf{k}$ space. For this purpose, we write the integral of Eq. (4.5) as the double integral over the entire 2D space

$$J(r,r') = \int_0^\infty dR R \int_0^\infty dR' R' \int_0^{2\pi} d\varphi \int_0^{2\pi} d\varphi' \delta(r-R) \times R^{-1} n_\alpha(\mathbf{R}) \left[\frac{\delta_{\alpha\beta}}{|\mathbf{R}-\mathbf{R}'|} - \nu \nabla_\alpha \nabla_\beta |\mathbf{R}-\mathbf{R}'| \right] \times n_\beta(\mathbf{R}') R'^{-1} \delta(r'-R'). \tag{4.6}$$

It should be noted that, in Eq. (4.6) R and R' are variables of the integration, whereas r and r' are parameters. We introduce the Fourier transformations

$$\tilde{\mathcal{N}}_\alpha(\mathbf{k};r) = \int d^2\mathbf{R} R^{-1} \delta(r-R) n_\alpha(\mathbf{R}) \exp(-i\mathbf{k}\cdot\mathbf{r}), \tag{4.7a}$$

$$\tilde{\mathcal{G}}_{\alpha\beta}(\mathbf{k}) = \int d^2\mathbf{R} \left[\frac{\delta_{\alpha\beta}}{|\mathbf{R}|} - \nu \nabla_\alpha \nabla_\beta |\mathbf{R}| \right] \exp(-i\mathbf{k}\cdot\mathbf{R}). \tag{4.7b}$$

To calculate the integral of Eq. (4.7a) we note that for an island having a conical shape, the surface projection of the normal vector

$$n_\alpha(\mathbf{R}) = \frac{R_\alpha}{R}\tan\vartheta. \tag{4.8}$$

Substituting Eq. (4.8) into Eq. (4.7a) and denoting the polar angle in the $\mathbf{R}$ space as φ, and the polar angle in the $\mathbf{k}$ space as ψ, one obtains

$$\tilde{\mathcal{N}}_\alpha(\mathbf{k};r) = \int_0^\infty dR R \int_0^{2\pi} d\varphi R^{-1} \delta(r-R) \tan\vartheta \frac{R_\alpha}{R} \times \exp[-ikR\cos(\varphi-\psi)]. \tag{4.9}$$

We now calculate the Fourier transform of the x–component of the normal vector ($\alpha=1$). The integration in Eq. (4.9) over R is trivial, and the integral reduces to

$$\tilde{\mathcal{N}}_x(\mathbf{k};r) = \tan\vartheta \int_0^{2\pi} d\varphi \cos\varphi \exp[-ikr\cos(\varphi-\psi)]. \tag{4.10}$$

Introducing a new variable $\chi \equiv \varphi - \psi$, the integral of Eq. (4.10) reduces to

$$\tilde{\mathcal{N}}_x(\mathbf{k};r) = \tan\vartheta \int_0^{2\pi} d\chi \cos(\chi+\psi) \exp[-ikr\cos\chi]. \tag{4.11}$$

After performing a standard transformation

$$\cos(\chi+\psi) = \cos\chi\cos\psi - \sin\chi\sin\psi, \tag{4.12}$$

and substituting this expression into Eq. (4.11), the integrand becomes a sum of the even and the odd functions of $(\cos\chi)$. The integral of the odd function vanishes, and the remaining integral yields

$$\begin{aligned} \tilde{\mathcal{N}}_x(\mathbf{k};r) &= \tan\vartheta\cos\psi \int_0^{2\pi} d\chi \cos\chi \exp[-ikr\cos\chi] \\ &= i\tan\vartheta\cos\psi \frac{d}{d(kr)} \int_0^{2\pi} d\chi \exp[-ikr\cos\chi] \\ &= i\tan\vartheta\cos\psi (2\pi) \frac{d}{d(kr)} J_0(kr) \\ &= -i\tan\vartheta\cos\psi (2\pi) J_1(kr) \\ &= -i\tan\vartheta \frac{k_x}{k} (2\pi) J_1(kr). \end{aligned} \tag{4.13}$$

The Fourier transform of the y-component of the normal vector can be calculated in the same way. Finally, one obtains

$$\tilde{\mathcal{N}}_\alpha(\mathbf{k};r) = -i(2\pi)\tan\vartheta\frac{k_\alpha}{k}J_1(kr). \tag{4.14}$$

To carry out the Fourier transformation in Eq. (4.7b), we note that

$$\int d^2\mathbf{R}\frac{1}{R}\exp(-i\mathbf{k}\cdot\mathbf{R}) = \frac{2\pi}{k}, \tag{4.15a}$$

$$\int d^2\mathbf{R}R\,\exp(-i\mathbf{k}\cdot\mathbf{R}) = -\frac{2\pi}{k^3} \tag{4.15b}$$

(see Appendix A). By substituting Eq. (4.15) into Eq. (4.7b), one obtains

$$\tilde{\mathcal{G}}_{\alpha,\beta}(\mathbf{k}) = \frac{2\pi}{k}\left[\delta_{\alpha\beta} - \nu\frac{k_\alpha k_\beta}{k^2}\right]. \tag{4.16}$$

The double integral in the real space in Eq. (4.6) can be written as the integral in the **k** space

$$J(r,r') = \int \frac{d^2\mathbf{k}}{(2\pi)^2}[\tilde{\mathcal{N}}_\alpha(\mathbf{k};r)]^*\tilde{\mathcal{G}}_{\alpha\beta}(\mathbf{k})\tilde{\mathcal{N}}_\beta(\mathbf{k};r'). \tag{4.17}$$

By substituting $\tilde{\mathcal{N}}_\alpha(\mathbf{k};r)$ from Eq. (4.14) and $\tilde{\mathcal{G}}_{\alpha\beta}(\mathbf{k})$ from Eq. (4.16) into Eq. (4.17), one obtains

$$J(r,r') = (2\pi)^2\frac{1}{(2\pi)^2}(2\pi)\int_0^\infty dk k\,\tan\vartheta\frac{k_\alpha}{k}J_1(kr)\frac{2\pi}{k} \times\left[\delta_{\alpha\beta} - \nu\frac{k_\alpha k_\beta}{k^2}\right]\tan\vartheta\frac{k_\beta}{k}J_1(kr'). \tag{4.18}$$

The integration over ψ is trivial and yields (2π). Thus, the integral of Eq. (4.18) reduces to

$$J(r,r') = (2\pi)^2[\tan\vartheta]^2(1-\nu)\int_0^\infty dk J_1(kr)J_1(kr'). \tag{4.19}$$

This integral has been calculated in Sec. III [see Eq. (3.7), the term in the sum with $m=1$]. Hence,

$$J(r,r') = (2\pi)^2[\tan\vartheta]^2(1-\nu) \times\left(\frac{r_<}{r_>^2}\right)\frac{\Gamma\left(\frac{3}{2}\right)}{\Gamma(2)\Gamma\left(\frac{1}{2}\right)}{}_2F_1\left[\frac{3}{2},\frac{1}{2};2;\left(\frac{r_<}{r_>}\right)^2\right]. \tag{4.20}$$

Substituting $J(r,r')$ from Eq. (4.20) into the expression for the elastic relaxation energy given by Eq. (4.4) yields

$$\Delta E_{\text{self}} = \frac{1}{2\pi}\frac{1+\nu}{1-\nu}W_0(2\pi)^2[\tan\vartheta]^2(1-\nu) \times\int_0^\rho dr r\int_0^\rho dr' r'\left(\frac{r_<}{r_>^2}\right)\frac{1}{2}{}_2F_1\left(\frac{3}{2},\frac{1}{2};2;(r_</r_>)^2\right). \tag{4.21}$$

It is possible to split the domain of integration in the double integral over r and r' in Eq. (4.21) into two subdomains, where $r>r'$ in one subdomain, and $r<r'$ in the other subdomain. The two integrals are equal, and ΔE_{self} from Eq. (4.21) equals twice the integral over one subdomain. By introducing variables $r_>=r$, and $r_<=r'$, Eq. (4.21) reduces to

$$\Delta E_{\text{self}} = 2(2\pi)(1+\nu)W_0[\tan\vartheta]^2\int_0^\rho dr_> r_> \times\int_0^{r_>} dr_< r_<\left(\frac{r_<}{r_>^2}\right)\frac{1}{2}{}_2F_1\left(\frac{3}{2},\frac{1}{2};2;(r_</r_>)^2\right). \tag{4.22}$$

Now, by introducing the variable $t=(r_</r_>)^2$, it is possible to write the double integral in Eq. (4.22) as the integral over $r_>$ and t:

$$\Delta E_{\text{self}} = (2\pi)2(1+\nu)W_0[\tan\vartheta]^2 \times\frac{1}{2}\frac{1}{2}\int_0^\rho dr_> r_>^2\int_0^1 dt t^{1/2}\,{}_2F_1\left(\frac{3}{2},\frac{1}{2};2;t\right). \tag{4.23}$$

An important feature of Eq. (4.23) is that the inner and outer integrals are uncoupled. The outer integral equals $(1/3)\rho^3$. By substituting the expression for the volume of the cone

$$V = \frac{1}{3}\tan\vartheta\pi\rho^3 \tag{4.24}$$

in Eq. (4.4), one obtains

$$\Delta E_{\text{self}} = (1+\nu)\tan\vartheta W_0 V\mathcal{J}, \tag{4.25}$$

where

$$\mathcal{J} = \int_0^1 dt t^{1/2}\,{}_2F_1\left(\frac{3}{2},\frac{1}{2};2;t\right). \tag{4.26}$$

V. NUMERICAL FACTOR IN THE ELASTIC RELAXATION ENERGY

To evaluate the numerical factor $\mathcal{J}$ in Eq. (4.26), we substitute the series expansion of the hypergeometric function ${}_2F_1(\frac{3}{2},\frac{1}{2};2;t)$ in the integrand. Hence,

$$\mathcal{J}=\int_0^1 dt\sum_{p=0}^{\infty}\frac{\Gamma\left(\frac{3}{2}+p\right)\Gamma\left(\frac{1}{2}+p\right)\Gamma(2)}{\Gamma\left(\frac{3}{2}\right)\Gamma\left(\frac{1}{2}\right)\Gamma(2+p)\Gamma(1+p)}t^{p+1/2}$$

$$=\sum_{p=0}^{\infty}\frac{\Gamma\left(\frac{3}{2}+p\right)\Gamma\left(\frac{1}{2}+p\right)\Gamma(2)}{\Gamma\left(\frac{3}{2}\right)\Gamma\left(\frac{1}{2}\right)\Gamma(2+p)\Gamma(1+p)}\frac{1}{p+\frac{3}{2}}. \quad (5.1)$$

Numerical evaluation of this series sum yields

$$\mathcal{J}=1.059. \quad (5.2)$$

It is interesting to compare this result with the result for the volume elastic relaxation of a square-based pyramid obtained by Duport *et al.*.[21] The elastic relaxation energy of a pyramid equals

$$\Delta E_{\text{self}}=-\frac{4}{\pi}(1+\nu)(\sqrt{2}-1)[1+\ln(1+\sqrt{2})]W_0V\tan\vartheta. \quad (5.3)$$

Numerical evaluation of the analytic expression given by Eq. (5.3) yields

$$\Delta E_{\text{self}}=-0.9922(1+\nu)W_0V\tan\vartheta. \quad (5.4)$$

The two numerical factors, one for a pyramid from Eq. (5.4), and the other for a cone from Eq. (5.2) are very close, as expected.

VI. ISLAND TOTAL ENERGY AND CHEMICAL POTENTIAL

The total formation energy of an island labeled i is the sum of the surface and strain energy $E_{i,\text{total}}=\Delta E_{i,\text{surf}}+\Delta E_{i,\text{el}}$ the effects of surface stress and the energy of the island edges being neglected.[5] For a conical island,

$$\Delta E_{i,\text{surf}}=\pi\rho_i^2[\gamma(\vartheta_i)\sec\vartheta_i-\gamma(0)]=\frac{3}{2}\beta V_i^{2/3}, \quad (6.1)$$

where $\gamma(\vartheta_i)$ and $\gamma(0)$ are the surface energies of the tilted surface of the island and of the flat surface of the wetting layer, respectively, with $\beta=2\pi^{1/3}3^{-1/3}(\cot\vartheta_i)^{2/3}[\gamma(\vartheta_i)\sec\vartheta_i-\gamma(0)]$.

The elastic energy is comprised of the self-relaxation energy and the interaction energy of the ith island with all other islands j. Hence $\Delta E_{i,\text{el}}=\Delta E_{i,\text{self}}+\Sigma_{j\neq i}E_{i,\text{inter}}^{(j)}$, where $E_{i,\text{inter}}^{(j)}$ is the interaction energy between islands i and j. From Eqs. (3.23) and (4.25) we have

$$\Delta E_{i,\text{el}}=-\alpha\mathcal{J}\tan\vartheta_i V_i+\frac{\alpha}{\pi}\sum_{j\neq i}\frac{V_iV_j}{R_{ij}^3}F\left(\frac{\rho_i}{R_{ij}},\frac{\rho_j}{R_{ij}}\right), \quad (6.2)$$

where $\alpha=(1+\nu)W_0$ and R_{ij} is the distance between the centers of the bases of the islands i and j.

To model the kinetics of Ostwald ripening or coarsening[4,9,11,12,15,22–24] it is important to know the chemical potential of the island i defined by

$$\mu_i=\Omega\frac{\partial E_{i,\text{total}}}{\partial V_i}, \quad (6.3)$$

where Ω is the atomic volume. The chemical potential has contributions corresponding to each of the energy terms discussed above,

$$\mu_i=\mu_{i,\text{surf}}+\mu_{i,\text{self}}+\sum_{j\neq i}\mu_{i,\text{inter}}^{(j)}. \quad (6.4)$$

From Eq. (6.1), $\mu_{i,\text{surf}}=\Omega\beta V_i^{-1/3}$, and from Eq. (4.25), $\mu_{i,\text{self}}=-\Omega\alpha J\tan\vartheta_i$. The term $\mu_{i,\text{inter}}^{(j)}$ is the contribution to the chemical potential of island i due to its interaction with island j, and is given by

$$\mu_{i,\text{inter}}^{(j)}=\Omega\left.\frac{\partial E_{i,\text{inter}}^{(j)}}{\partial V_i}\right|_{\substack{V_j=\text{const}\\ \tan(\vartheta_i)=\text{const}\\ \tan(\vartheta_j)=\text{const}}}. \quad (6.5)$$

By substituting the interaction energy from Eq. (3.23) into Eq. (6.5), and by using the identity

$$\frac{\partial F(\eta_i,\eta_j)}{\partial V_i}=\frac{1}{V_i}\frac{\frac{d\rho_i}{\rho_i}\frac{d\eta_i}{\eta_i}}{\frac{dV_i}{V_i}\frac{d\rho_i}{\rho_i}}\eta_i\frac{\partial F(\eta_i,\eta_j)}{\partial\eta_i}, \quad (6.6)$$

one obtains

$$\mu_{i,\text{inter}}^{(j)}=\Omega\frac{\alpha}{\pi}V_j\frac{1}{R_{ij}^3}\left[F\left(\frac{\rho_i}{R_{ij}};\frac{\rho_j}{R_{ij}}\right)+\frac{1}{3}G\left(\frac{\rho_i}{R_{ij}};\frac{\rho_j}{R_{ij}}\right)\right]. \quad (6.7)$$

Here

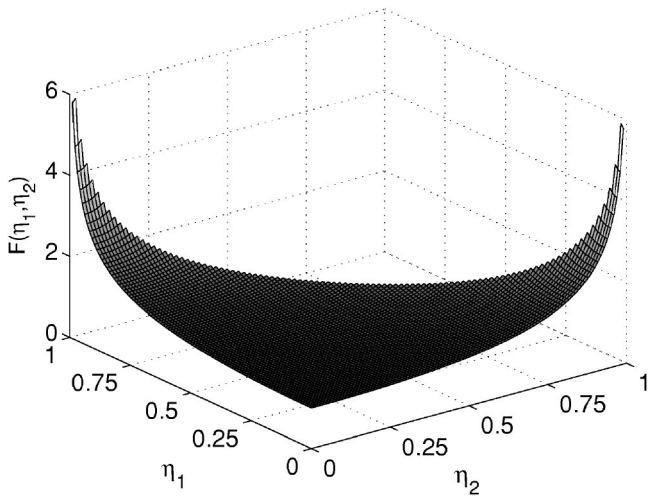

FIG. 1. The function $F(\eta_1,\eta_2)$.

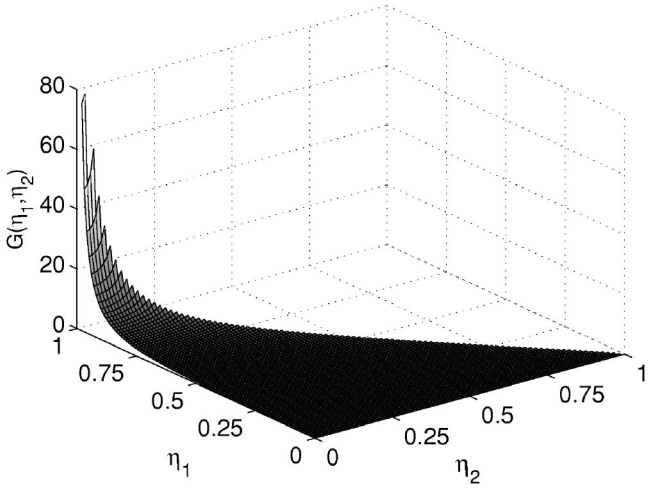

FIG. 2. The function $G(\eta_1, \eta_2)$.

$$G\left(\frac{\rho_i}{R_{ij}};\frac{\rho_j}{R_{ij}}\right) \equiv \eta_i \frac{\partial F(\eta_i,\eta_j)}{\partial \eta_i} = \sum_{s=0}^{\infty}\left\{\left[\frac{\Gamma\left(\frac{3}{2}+s\right)}{\Gamma\left(\frac{3}{2}\right)}\right]^2 \times \sum_{p=0}^{s} 2p\left[\frac{\eta_i^p \eta_j^{s-p}}{\Gamma(p+1)\Gamma(s-p+1)}\right]^2 \times \frac{\frac{3}{2}}{(p+1)\left(p+\frac{3}{2}\right)} \frac{\frac{3}{2}}{(s-p+1)\left(s-p+\frac{3}{2}\right)}\right\}. \tag{6.8}$$

The functions $F(\eta_i, \eta_j)$ and $G(\eta_i, \eta_j)$ are defined for

$$0 \leqslant \eta_i \leqslant 1, \quad 0 \leqslant \eta_j \leqslant 1, \quad \eta_i + \eta_j \leqslant 1, \tag{6.9}$$

and can be evaluated over the entire domain of definition and stored in the form of a look-up table to be accessed in simulations of island ripening kinetics. Calculated values for F and G are displayed in Figs. 1 and 2, respectively. The function F indicates the factor by which the interaction energy deviates from the dipole-dipole approximation [Eq. (3.23)]. It converges over the entire domain of definition indicated in Eq. (6.9). For remote islands, when $\eta_{1,2} \to 0$, F equals unity and the dipole-dipole model is a good approximation. As the islands tend to touch $(\eta_1 + \eta_2 \to 1)$, F increases rapidly, diverging from the dipole-dipole approximation. The results for the function G are divergent for $\eta_1 \to 1$.

VII. CONCLUSIONS

We have employed projection force density methods and the surface Green's function for isotropic solids to obtain elastic self-relaxation and interaction energies for coherently strained conical islands. These expressions are used to evaluate the island chemical potential which can form the basis for models of strained island coarsening[15] and stability.[13] The work could be further extended, for example, to investigate island shape transformations in the presence of elastic interactions and the influence of island interactions on the spatial variation of the adatom chemical potential. The advantage of the method proposed in the present paper in dynamical simulations of island evolution is that with a suitable tabulation of functions, the effect of elastic interactions can be included using a simple look-up table.

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APPENDIX A

This appendix contains some useful Fourier transformations employed in the analysis. Consider

$$\int d^2\mathbf{r}\frac{1}{r}\exp(-i\mathbf{k}\cdot\mathbf{r}) = \int_0^{\infty} dr r \frac{1}{r}\int_0^{2\pi} d\varphi \exp(-ikr\cos\varphi) = 2\pi\int_0^{\infty} dr J_0(kr) = \frac{2\pi}{k}. \tag{A1}$$

Thus,

$$F\left\{\frac{1}{r}\right\} = \frac{2\pi}{k}. \tag{A2}$$

Consider now

$$F\{r\} \equiv \int d^2\mathbf{r}\, r \exp(-i\mathbf{k}\cdot\mathbf{r}). \tag{A3}$$

The integral (A3) diverges, but can be regarded as a generalized function. We note that

$$\nabla^2 r = \frac{1}{r}\left(\frac{d}{dr} r \frac{d}{dr} r\right) = \frac{1}{r}. \tag{A4}$$

Now, writing the same identity for Fourier transforms, we obtain

$$F\{\nabla^2 r\} = -k^2 F\{r\} = F\left\{\frac{1}{r}\right\}. \tag{A5}$$

By substituting Eq. (A2) into Eq. (A5), we finally obtain

$$F\{r\} = -\frac{2\pi}{k^3}. \tag{A6}$$

APPENDIX B

By using Eq. (A2), we write $|\mathbf{r}-\mathbf{r}'|^{-1}$ as the inverse Fourier integral

$$\frac{1}{|\mathbf{r}-\mathbf{r}'|} = \int_0^\infty \frac{dkk}{(2\pi)^2}\frac{2\pi}{k}\int_0^{2\pi} d\psi \exp[i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')]$$
$$= \int_0^\infty \frac{dk}{2\pi}\int_0^{2\pi} d\psi \exp[ikr\cos(\varphi-\psi)]$$
$$\times\exp[ikr'\cos(\varphi'-\psi)]. \quad \text{(B1)}$$

Here φ, φ', and ψ are polar angles of the position vectors $\mathbf{r}$, $\mathbf{r}'$, and the wave vector $\mathbf{k}$, respectively. Now we expand each of the exponentials in the integrand of Eq. (B1) in a Fourier series

$$\exp[ikr\cos(\varphi-\psi)] = \sum_{m=-\infty}^{\infty} a_m \exp(im\psi). \quad \text{(B2)}$$

We find the coefficients a_m of the expansion Eq. (B2) as follows:

$$a_m = \frac{1}{2\pi}\int_0^{2\pi} d\psi \exp[ikr\cos(\varphi-\psi)]\exp[-im\psi]$$
$$= \frac{1}{2\pi}\exp(-im\varphi)\int_0^{2\pi} d\psi \exp[ikr\cos(\varphi-\psi)]$$
$$\times\exp[im(\varphi-\psi)] = \exp[-im\psi]J_m(kr). \quad \text{(B3)}$$

By substituting the coefficients a_m from Eq. (B3) and by performing integration over ψ, one obtains Eq. (3.6).

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