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Misfit dislocation loops in composite nanowires

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ABSTRACT

A new mechanism for relaxation of misfit stresses in composite nanowires (quantum wires) is suggested and theoretically examined, namely the formation of misfit dislocation loops. The stress field of a prismatic dislocation loop in a cylinder (nanowire) is calculated. The parameters of two-phase composite nanowires at which the formation of misfit dislocation loops is energetically favourable are estimated. The effect of stress fields of dislocation loops on the formation of compositionally modulated nanowires is discussed.

§ 1. INTRODUCTION

Nanowires with their unique physical properties represent the subject of growing fundamental research motivated by a range of new applications (for example Cui and Lieber (2001), Langlais *et al.* (2001), Ovid'ko and Sheinerman (2001), Priester and Grenet (2001), Gudiksen *et al.* (2002), Lauhon *et al.* (2002) and Wang *et al.* (2002)). Of special interest is the behaviour of composite (two-phase) nanowires such as nanowires in 'shells' (Lauhon *et al.* 2002) and compositionally modulated nanowires (Priester and Grenet 2001), because of their importance for high technologies based on nanostructures with complicated architecture as well as for understanding the nature of nanoscale effects in composite solids. With the two-phase structure of these nanowires, interphase boundaries are expected to play an essential role in physical processes occurring in the nanowires. In particular, misfit dislocations are capable of being generated in composite nanowires, strongly affecting their functional properties. Although we are as yet unaware of any experimental observations of misfit dislocations in nanowires, we suppose that such dislocations may form in composite nanowires much as they are generated in flat thin films and quantum dots (for example Fitzgerald (1991), Jain *et al.* (1997), Liu *et al.* (2000), Ovid'ko (2002) and Ovid'ko and Sheinerman (2002)). In the paper by Gutkin *et al.* (2000), conventional straight misfit dislocations in two-phase composite solids having the wire form (nanowires in 'shells') have been theoretically examined. The main aim of this paper is to suggest a theoretical model describing misfit dislocation configurations of the new type in two-phase composite nanowires, namely the misfit dislocation loops in nanowires embedded in 'shells' (figure 1).

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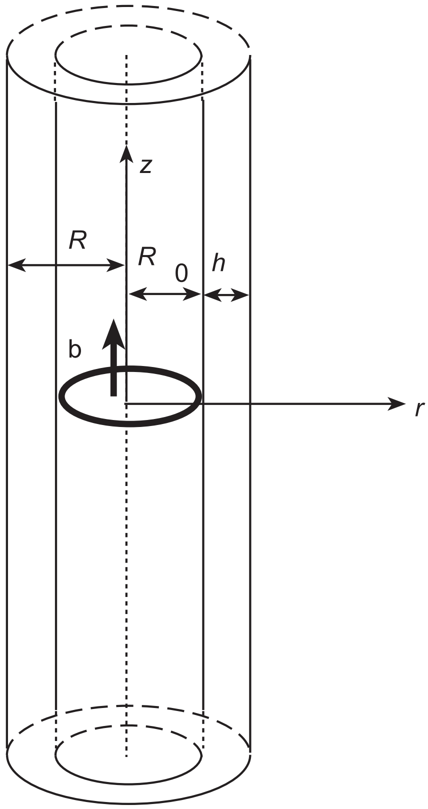


Figure 1. Prismatic misfit dislocation loop in a two-phase composite cylinder (nanowire).

§ 2. Composite nanowire with misfit dislocation loops: model

Let us consider a two-phase composite nanowire as a composite cylinder with radius R and infinite length. The model cylinder is composed of an internal cylinder (substrate) of radius $R_0 < R$ and a film of thickness $h = R - R_0$, which envelops the internal cylinder as shown in figure 1. In the framework of the suggested first approximation model, we shall not take into account the crystallography of the adjacent film and substrate, in which case the interphase (film–substrate) boundary is treated as a surface of the internal cylinder (figure 1). (That is, there are no facets at the interphase boundary.)

The film and substrate are assumed to be isotropic solids having the same values of the shear modulus G and the same values of Poisson's ratio ν. The film–substrate boundary is characterized by the two-dimensional dilatation misfit parameter $f = 2(a_2 - a_1)/(a_2 + a_1)$, where a_1 and a_2 are the crystal lattice parameters of the substrate and the film respectively.

Misfit stresses occur in film/substrate composite solids owing to the geometric mismatch characterized by f at interphase boundaries between crystalline lattices of films and substrates. In most cases, a partial relaxation of the misfit stresses is realized via generation of various defects (for example Fitzgerald (1991), Jain *et al.* (1997), Müllner *et al.* (1997) and Gao *et al.* (1999)). The conditions at which isolated misfit dislocations (MDs), misfit disclinations and their configurations (dipoles, rows and walls) are generated in wire composite solids have been analysed

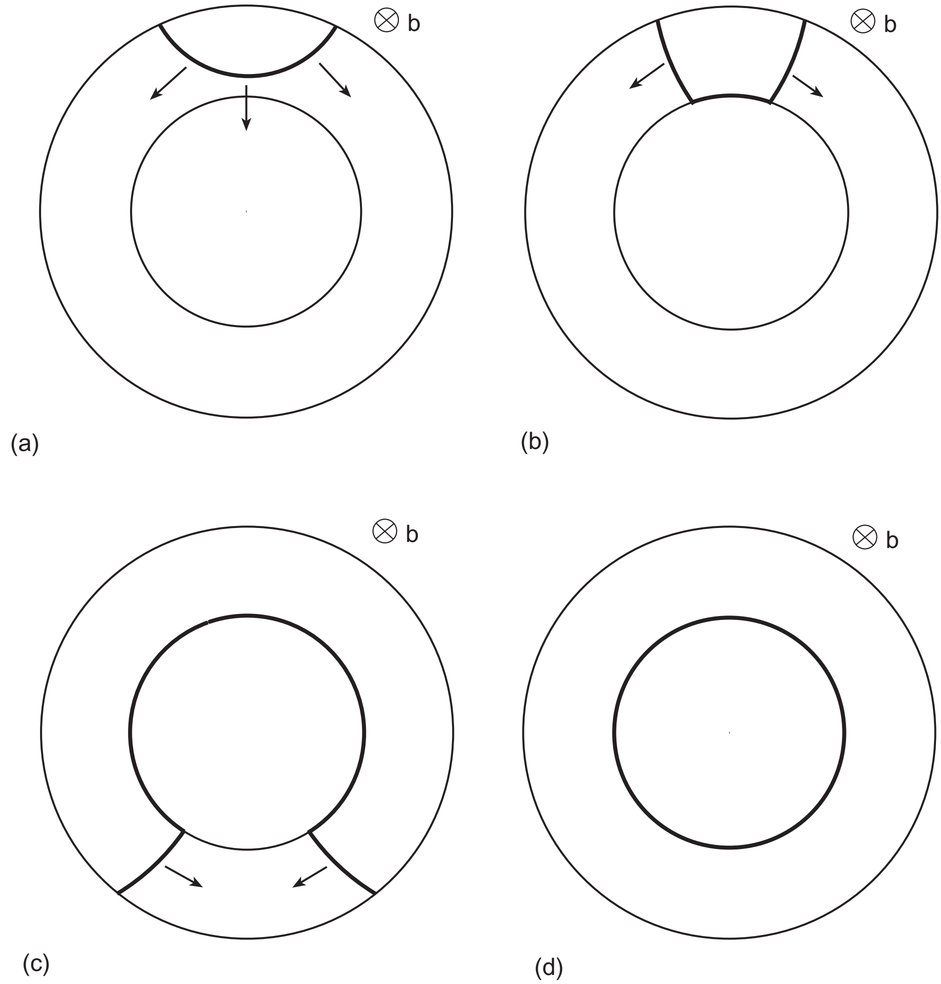


Figure 2. Climb mechanism for formation of a MD loop in a two-phase composite nanowire. ***b*** denotes the dislocation Burgers vector.

by Gutkin *et al*. (2000) and Sheinerman and Gutkin (2001). In this paper we elaborate a theoretical model describing the formation of prismatic MD loops (figure 2), MD configurations of the new type in composite nanowires, whose stress fields can induce modulation of the chemical composition of the nanowires.

In general, there are several potential mechanisms for the formation of MD loops in composite nanowires. A prismatic MD loop can be formed, for instance, through generation of a dislocation semiloop at the lateral free surface of the nanowire (figure 2 (a)), its climb towards the interphase boundary (figure 2 (b)), its consequent expansion in the plane of the cylinder cross-section (figure 2 (c)), and merging and annihilation of two opposite-sign MD segments between the interphase boundary and the nanowire free surface (figure 2 (d)). The nucleation of a dislocation semiloop occurs at the lateral free surface of the nanowire (figure 2 (a)), where the semiloop is the easiest to generate at a stress concentrator, for example at a surface step. Also, the expansion of the semiloop in the plane of the nanowire cross-section is

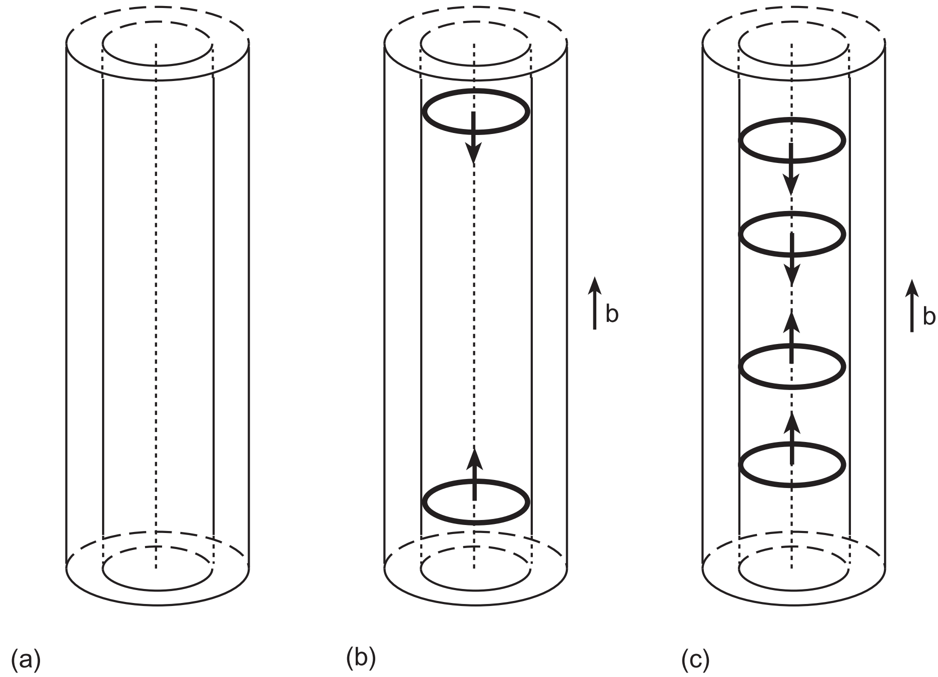


Figure 3. Glide mechanism for formation of MD loops in a two-phase composite nanowire: (a) nanowire in its initial dislocation-free state; (b), (c) generation of prismatic dislocation loops at the upper and bottom free surfaces of the nanowire and their consequent glide towards the central area of the nanowire. ***b*** denotes the dislocation Burgers vector.

realized by climb (figure 2). Therefore, it is a rather slow process whose velocity is controlled by point-defect migration associated with dislocation climb.

Besides the climb mechanism (figure 2), there is also a glide mechanism for the formation of MD loops (figure 3). Prismatic MD loops are generated at the upper and bottom free surfaces of a composite nanowire of finite length and then glide towards the central area of the nanowire (figure 3). The action of this glide mechanism is effective, in particular, in short nanowires.

Both the mechanisms for the formation of MD loops (figures 2 and 3) can be simultaneously realized in a composite nanowire (figure 4). In doing so, the climb mechanism is dominant in the central area of the nanowire, while the upper and bottom free surfaces of the nanowire serve as effective sources of gliding MD loops (figure 4).

Now let us analyse the conditions in which the formation of a prismatic MD loop at the interphase boundary is energetically favourable in a cylindrical composite nanowire (figure 1). To do this, we shall calculate and compare energy characteristics of two physical states realized in a composite nanowire, namely the coherent state with MD-free interphase boundary and the semicoherent state with the interphase boundary containing one MD loop, which accommodates, in part, the misfit stresses. The formation of the first MD loop is energetically favourable, if it leads to a decrease in the total energy, that is if the energy difference ΔW between the final and initial states is negative. ΔW consists of the three terms, in which case we have

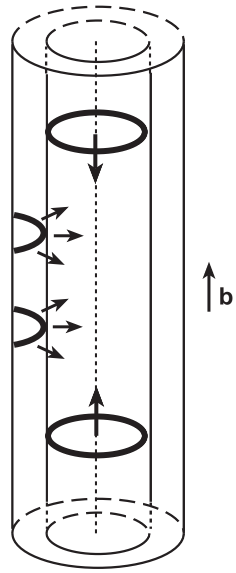


Figure 4. Combined action of the climb and glide mechanisms for formation of MD loops in a two-phase composite nanowire. ***b*** denotes the dislocation Burgers vector.

the following criterion for the formation of the MD loop to be energetically favourable:

$$\Delta W = W^{l} + W^{l-f} + W^{c} < 0. \tag{1}$$

Here W^{l} denotes the proper elastic energy of the MD loop, W^{l-f} the energy that characterizes the elastic interaction between the MD loop and the misfit stresses, and W^{c} the energy of the MD loop core. In order to calculate W^{l} and W^{l-f}, in the following section we shall calculate the stress fields created by a MD loop in a cylindrical composite solid (nanowire).

§ 3. Stress field of a misfit dislocation loop in two-phase composite nanowire

The problems of calculation of elastic fields of circular dislocation loops have been addressed by many workers. To date, solutions have been obtained for circular dislocation loops in an isotropic infinite medium (Kröner 1958, Kroupa 1960, 1962a,b, Bullough and Newmann 1960, Marchikowsky and Sree Harsha 1968, Huang and Mura 1970, Demir *et al.* 1992, Khraishi *et al.* 2000a,b, Kolesnikova and Romanov 2003), isotropic half-spaces (Baštecká 1964, Jäger *et al.* 1975, Ohr 1978), two-phase composite materials with a planar interphase boundary (Salamon and Dundurs 1971, 1977, Dundurs and Salamon 1972, Salamon and Comninou 1979, Salamon 1981, Yu and Sanday 1991), isotropic (Chou 1963) and anisotropic (Chou 1964) plate and an elastic sphere (Willis *et al.* 1983). However, the solutions that have been available up until now are not suitable for the calculation of energies of dislocation loops in nanowires. Therefore, in this section, we calculate the stress field of a circular prismatic dislocation loop in an elastically isotropic cylinder.

Let us introduce the cylindrical coordinate system (r, θ, z) with the z axis being the central line of the cylinder (figure 1). Let the centre of the MD loop be located at the centre line $r = 0$ of the cylinder, which plays the role of the symmetry axis. The MD loop is located in the plane $z = 0$ and has the radius R_0 and Burgers vector $\boldsymbol{b} = b_z \boldsymbol{e}_z$. In the framework of our model, the cylindrical composite nanowire with a prismatic dislocation loop has its centre line as the symmetry axis.

In our calculations of the stress field σ_{ij}^{l} of a MD loop in a cylindrical composite (figure 1), we shall use the expressions (Dundurs and Salamon 1972, Salamon and Comninou 1979, Kolesnikova and Romanov 2003) for the stress fields of MD loops in elastically isotropic infinite media. In doing this, we represent the stress field σ_{ij}^{l} as the following sum: $\sigma_{ij}^{\mathrm{l}} = \sigma_{ij}^{\infty} + \sigma_{ij}^{\mathrm{v}}$, where σ_{ij}^{∞} is the stress field created by the MD loop in an infinite medium and σ_{ij}^{v} is the additional stress field that allows one to satisfy the boundary conditions at the cylinder free surface $r = R$. These boundary conditions are as follows: $\sigma_{rk}^{\infty}(r = R) + \sigma_{rk}^{\mathrm{v}}(r = R) = 0$, where $k = r, \theta, z$.

The stress field σ_{ij}^{∞} has been given by Dundurs and Salamon (1972), Salamon and Comninou (1979), Kolesnikova and Romanov (2003) as

$$\sigma_{rr}^{\infty} = -M\left(\frac{1-2\nu}{\tilde{r}}J(1,1;0) + |\tilde{z}|J(1,0;2) - J(1,0;1) - \frac{|\tilde{z}|}{\tilde{r}}J(1,1;1)\right), \tag{2}$$

$$\sigma_{\theta\theta}^{\infty} = -M\left(\frac{2\nu-1}{\tilde{r}}J(1,1;0) - 2\nu J(1,0;1) + \frac{|\tilde{z}|}{\tilde{r}}J(1,1;1)\right), \tag{3}$$

$$\sigma_{zz}^{\infty} = M[J(1,0;1) + |\tilde{z}|J(1,0;2)], \tag{4}$$

$$\sigma_{rz}^{\infty} = M\tilde{z}J(1,1;2), \tag{5}$$

$$\sigma_{r\theta}^{\infty} = \sigma_{z\theta}^{\infty} = 0. \tag{6}$$

Here $\tilde{r} = r/R_0$, $\tilde{z} = z/R_0$, $M = Gb_z/2(1-\nu)R_0$ and $J(m,n;p)$ are the Lipschitz–Hankel integrals. They are defined (Eason *et al.* 1955) as $J(m,n;p) = \int_0^{\infty} J_m(t) J_n(\tilde{r}t) \exp(-|\tilde{z}|t)\, t^p\, \mathrm{d}t$, with $J_m(t)$ being the first-type Bessel functions of the mth order.

The strained state of a two-phase composite cylinder is characterized by the absence of torsion. In this situation, the stress field σ_{ij}^{v} does not depend on θ, and its components $\sigma_{r\theta}^{\mathrm{v}}$ and $\sigma_{z\theta}^{\mathrm{v}}$ are equal to zero. For this stress field, one can introduce the stress function φ, satisfying equation (Timoshenko and Goodier 1970) $\Delta\Delta\varphi = 0$, where Δ denotes the Laplace operator. This operator is written in cylindrical coordinates as $\Delta = \partial^2/\partial r^2 + (1/r)(\partial/\partial r) + (1/r^2)(\partial^2/\partial\theta^2) + \partial^2/\partial z^2$. For the stress function φ which does not depend on θ, we obtain $\Delta\varphi = (\partial^2\varphi/\partial r^2) + (1/r)(\partial\varphi/\partial r) + \partial^2\varphi/\partial z^2$. The stress tensor components σ_{ij}^{v} are expressed through the stress function φ by the following relationships (Timoshenko and Goodier 1970):

$$\sigma_{rr}^{\mathrm{v}} = \frac{\partial}{\partial z}\left(\nu\,\Delta\varphi - \frac{\partial^2\varphi}{\partial r^2}\right), \quad \sigma_{\theta\theta}^{\mathrm{v}} = \frac{\partial}{\partial z}\left(\nu\Delta\varphi - \frac{1}{r}\frac{\partial\varphi}{\partial r}\right), \tag{7}$$

$$\sigma_{zz}^{\mathrm{v}} = \frac{\partial}{\partial z}\left[(2-\nu)\Delta\varphi - \frac{\partial^2\varphi}{\partial z^2}\right], \quad \sigma_{rz}^{\mathrm{v}} = \frac{\partial}{\partial r}\left[(1-\nu)\Delta\varphi - \frac{\partial^2\varphi}{\partial z^2}\right], \tag{8}$$

$$\sigma_{r\theta}^{\mathrm{v}} = \sigma_{z\theta}^{\mathrm{v}} = 0. \tag{9}$$

Note that σ_{rr}^{∞} and σ_{rz}^{∞} are even and odd functions respectively of $\tilde{z}$. Since the stresses σ_{rr}^{v} and σ_{rz}^{v} are in the relationships $\sigma_{rr}^{\mathrm{v}}(\tilde{r} = \tilde{R}) = -\sigma_{rr}^{\infty}(\tilde{r} = \tilde{R})$ and $\sigma_{rz}^{\mathrm{v}}(\tilde{r} = \tilde{R}) = -\sigma_{rz}^{\infty}(\tilde{r} = \tilde{R})$ (where $\tilde{R} = R/R_0$) with the stresses σ_{rr}^{∞} and σ_{rz}^{∞}, these stresses σ_{rr}^{v} and σ_{rz}^{v} are even and odd functions respectively of $\tilde{z}$. As a corollary, with the first formula from equations (7) and the second formula from equations (8), we find that φ is an odd function of $\tilde{z}$.

In the situation with a two-phase nanowire modelled as a composite cylinder of infinite length, the stress function φ being an odd function of $\tilde{z}$ can be represented in the following form (Timoshenko and Goodier 1970):

$$\varphi = MR_0^3 \int_0^\infty \Big[\rho_1(k) I_0(\tilde{r}k) - \tilde{r}k\rho_2(k) I_1(\tilde{r}k)\Big] \sin(k\tilde{z})\,\mathrm{d}k. \tag{10}$$

Here $I_0(\tilde{r}k)$ and $I_1(\tilde{r}k)$ are the modified Bessel functions of the zero order and first order, respectively; $\rho_1(k)$ and $\rho_2(k)$ are the functions determined from the boundary conditions.

With equations (7) and (8) substituted into equation (10), we have

$$\sigma_{rr}^{\mathrm{v}} = M\int_0^\infty \left[\left(-I_0(\tilde{r}k) + \frac{I_1(\tilde{r}k)}{\tilde{r}k}\right)\rho_1(k) + \Big[(1-2\nu)I_0(\tilde{r}k) + \tilde{r}kI_1(\tilde{r}k)\Big]\rho_2(k)\right] \times k^3\cos(k\tilde{z})\,\mathrm{d}k, \tag{11}$$

$$\sigma_{\theta\theta}^{\mathrm{v}} = M\int_0^\infty \left(-\frac{I_1(\tilde{r}k)}{\tilde{r}k}\rho_1(k) + (1-2\nu)I_0(\tilde{r}k)\rho_2(k)\right)k^3\cos(k\tilde{z})\,\mathrm{d}k, \tag{12}$$

$$\sigma_{zz}^{\mathrm{v}} = M\int_0^\infty \left\{I_0(\tilde{r}k)\rho_1(k) - \Big[2(2-\nu)I_0(\tilde{r}k) + \tilde{r}kI_1(\tilde{r}k)\Big]\rho_2(k)\right\}k^3\cos(k\tilde{z})\,\mathrm{d}k, \tag{13}$$

$$\sigma_{rz}^{\mathrm{v}} = M\int_0^\infty \left\{I_1(\tilde{r}k)\rho_1(k) - \Big[2(1-\nu)I_1(\tilde{r}k) + \tilde{r}kI_0(\tilde{r}k)\Big]\rho_2(k)\right\}k^3\sin(k\tilde{z})\,\mathrm{d}k. \tag{14}$$

In order to determine the functions $\rho_1(k)$ and $\rho_2(k)$ in the expressions for σ_{ij}^{v}, let us introduce the following functions:

$$g_1(\tilde{r},k) = \left[\left(-I_0(\tilde{r}k) + \frac{I_1(\tilde{r}k)}{\tilde{r}k}\right)\rho_1(k) + \Big[(1-2\nu)I_0(\tilde{r}k) + \tilde{r}kI_1(\tilde{r}k)\Big]\rho_2(k)\right]k^3, \tag{15}$$

$$g_2(\tilde{r},k) = \left\{I_1(\tilde{r}k)\rho_1(k) - \Big[2(1-\nu)I_1(\tilde{r}k) + \tilde{r}kI_0(\tilde{r}k)\Big]\rho_2(k)\right\}k^3. \tag{16}$$

In doing this, we shall search for g_1 and g_2 as even and odd functions, respectively, of k. Note that the stresses σ_{rr}^{v} and σ_{rz}^{v} in the situation discussed represent (with accuracy up to factors π and $-i\pi$) the inverse Fourier transforms of the functions g_1 and g_2: $\sigma_{rr}^{\mathrm{v}}(\tilde{r},\tilde{z}) = \pi F^{-1}[g_1]$, $\sigma_{rz}(\tilde{r},\tilde{z}) = -\mathrm{i}\pi F^{-1}[g_2]$, where $\mathrm{i} = -1^{1/2}$, and $F^{-1}[g](k) = (1/2\pi)\int_{-\infty}^{\infty} g(k)\exp(\mathrm{i}k\tilde{z})\,\mathrm{d}k$ is the inverse Fourier transform. In these circumstances, the inverse Fourier transform of $g_1(\tilde{r},k)$ (being an even function of k) and $g_2(\tilde{r},k)$ (being an odd function of k) are, respectively, as follows: $F^{-1}[g_1] = (1/\pi)\int_0^\infty g_1(\tilde{r},k)\cos(k\tilde{z})\,\mathrm{d}k$ and $F^{-1}[g_2] = (\mathrm{i}/\pi)\int_0^\infty g_2(\tilde{r},k)\sin(k\tilde{z})\,\mathrm{d}k$. Application of the direct Fourier transform $F[g](k) = \hat{g}(k) = \int_{-\infty}^{\infty} g(\tilde{z})\exp(-\mathrm{i}k\tilde{z})\,\mathrm{d}k$ to the stresses $\sigma_{rr}^{\mathrm{v}}(\tilde{r},\tilde{z})$ and $\sigma_{rz}^{\mathrm{v}}(\tilde{r},\tilde{z})$ yields

$$g_1(\tilde{r},k) = \frac{1}{\pi}\hat{\sigma}_{rr}^{\mathrm{v}}(\tilde{r},k), \quad g_2(\tilde{r},k) = \frac{\mathrm{i}}{\pi}\hat{\sigma}_{rz}^{\mathrm{v}}(\tilde{r},k). \tag{17}$$

Application of the direct Fourier transform to the boundary conditions $\sigma_{rr}^{\mathrm{v}}(\tilde{R},\tilde{z}) = -\sigma_{rr}^{\infty}(\tilde{R},\tilde{z})$ and $\sigma_{rz}^{\mathrm{v}}(\tilde{R},\tilde{z}) = -\sigma_{rz}^{\infty}(\tilde{R},\tilde{z})$ gives

$$\hat{\sigma}_{rr}^{\mathrm{v}}(\tilde{R},k) = -\hat{\sigma}_{rr}^{\infty}(\tilde{R},k), \quad \hat{\sigma}_{rz}^{\mathrm{v}}(\tilde{R},k) = -\hat{\sigma}_{rz}^{\infty}(\tilde{R},k). \tag{18}$$

From equations (17) and (18) we find that

$$g_1(\tilde{R},k) = -\frac{1}{\pi}\hat{\sigma}_{rr}^{\infty}(\tilde{R},k), \quad g_2(\tilde{R},k) = -\frac{\mathrm{i}}{\pi}\hat{\sigma}_{rz}^{\infty}(\tilde{R},k). \tag{19}$$

With equations (15) and (16) substituted into equation (19), we obtain the following system of equations for the functions $\rho_1(k)$ and $\rho_2(k)$:

$$a_{11}\rho_1 + a_{12}\rho_2 = b_1, \tag{20}$$

$$a_{21}\rho_1 + a_{22}\rho_2 = b_2. \tag{21}$$

Here

$$a_{11} = -I_0(\tilde{R}k) + \frac{I_1(\tilde{R}k)}{\tilde{R}k}, \tag{22}$$

$$a_{12} = (1-2\nu)I_0(\tilde{R}k) + \tilde{R}kI_1(\tilde{R}k), \tag{23}$$

$$a_{21} = I_1(\tilde{R}k), \tag{24}$$

$$a_{22} = -[2(1-\nu)I_1(\tilde{R}k) + \tilde{R}kI_0(\tilde{R}k)], \tag{25}$$

and the coefficients b_1 and b_2 are expressed through $\hat{\sigma}_{rr}^{\infty}(\tilde{R},k)$ and $\hat{\sigma}_{rz}^{\infty}(\tilde{R},k)$ by the following relationships: $b_1 = -1/(M\pi k^3)\hat{\sigma}_{rr}^{\infty}(\tilde{R},k)$, $b_2 = -\mathrm{i}/(M\pi k^3)\hat{\sigma}_{rr}^{\infty}(\tilde{R},k)$. Substitution of the expressions for $\hat{\sigma}_{rr}^{\infty}(\tilde{R},k)$ and $\hat{\sigma}_{rz}^{\infty}(\tilde{R},k)$ (derived in appendix A), into the above relationships gives

$$b_1 = \frac{2\,\mathrm{sgn}\,k}{\pi k^2}\left\{I_1(|k|)\left[\left(\tilde{R}|k| + \frac{2(1-\nu)}{\tilde{R}|k|}\right)K_1(\tilde{R}|k|) + K_0(\tilde{R}|k|)\right]\right.$$
$$\left. - |k|I_0(|k|)\left(K_0(\tilde{R}|k|) + \frac{K_1(\tilde{R}|k|)}{\tilde{R}|k|}\right)\right\}, \tag{26}$$

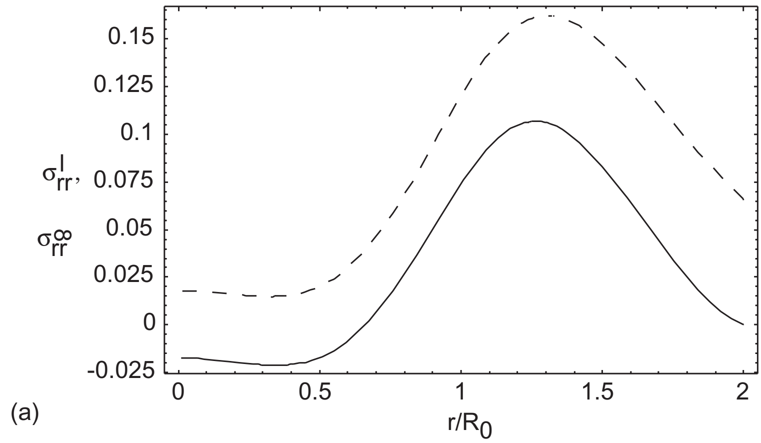
$$b_2 = \frac{2}{\pi|k|}\left\{\tilde{R}I_1(|k|)K_0(\tilde{R}|k|) - I_0(|k|)K_1(\tilde{R}|k|)\right\}. \tag{27}$$

Solution of the system (20) and (21) is as follows:

$$\rho_1 = \frac{b_1a_{22} - b_2a_{12}}{a_{11}a_{22} - a_{12}a_{21}}, \quad \rho_2 = \frac{b_2a_{11} - b_1a_{21}}{a_{11}a_{22} - a_{12}a_{21}}. \tag{28}$$

Since the function $I_0(\tilde{R}k)$ is even and the function $I_1(\tilde{R}k)$ is odd, from equations (15), (16) and (22)–(28) we find the condition that the function $g_1(k)$ is even and the function $g_2(k)$ is odd (see above) to be valid. In this situation, the stress field σ_{ij}^{v} is given by equations (9), (11)–(14) and (22)–(28). The sum stress field of the MD loop in a composite nanowire (figure 1) represents the sum of the stresses σ_{ij}^{∞} (given by equations (2)–(6)) and σ_{ij}^{v}.

For illustration, the dependences of the stresses σ_{rr}^{1} and σ_{rz}^{1} (in units of $Gb_z/2(1-\nu)R_0$) on r/R_0 are presented in figure 5, for $\tilde{z}=1$, $\tilde{R}=2$ and $\nu = 0.3$. The stresses σ_{rr}^{∞} and σ_{rz}^{∞} are shown as dashed curves in this figure. As follows from figure 5, the stresses σ_{rr}^{1} and σ_{rz}^{1} satisfy the boundary conditions at the cylinder (nanowire) free surface and are essentially different from the stresses σ_{rr}^{∞} and σ_{rz}^{∞}, respectively, which are created by a prismatic dislocation loop in an infinite medium.



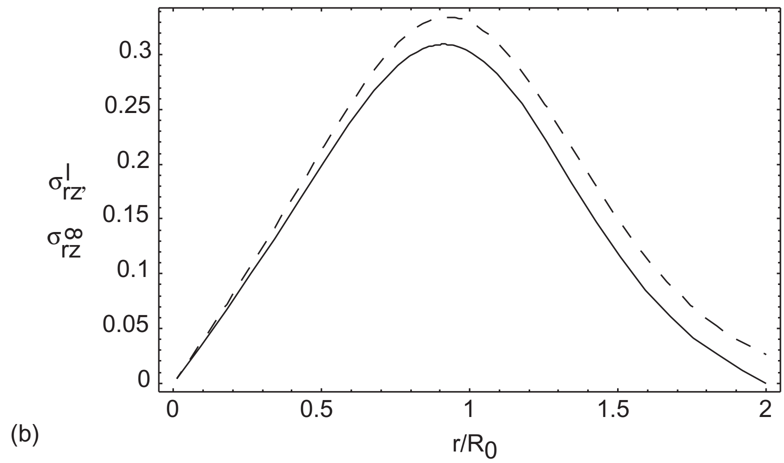


Figure 5. Dependences of stresses σ^{1}_{rr}, σ^{1}_{rz}, σ^{∞}_{rr} and σ^{∞}_{rz} on r/R_0, for $z/R_0 = 1$, $R/R_0 = 2$ and $\nu = 0.3$: (a) dependences $\sigma^{1}_{rr}(r/R_0)$ (——) and $\sigma^{\infty}_{rr}(r/R_0)$ (- - - -); (b) dependences $\sigma^{1}_{rz}(r/R_0)$ (——) and $\sigma^{\infty}_{rz}(r/R_0)$ (- - - - -).

§4. Critical condition for energetically favourable formation of a misfit dislocation loop in composite nanowire

With the stress field σ^{1}_{ij} calculated in § 3, we shall calculate the difference ΔW between the energy of the state of a composite nanowire with the MD loop (figure 1) and that of the defect-free state. In doing this, let us calculate terms W^{1}, $W^{1-\mathrm{f}}$ and W^{c} on the right-hand side of equation (1) for ΔW. The proper energy W^{1} is calculated using the general formula (Mura 1968)

$$W^{1} = \frac{b_z}{2} \int_0^{2\pi} \int_0^{R_0 - r_{\mathrm{c}}} \sigma^{1}_{zz}(\tilde{r}, \tilde{z} = 0) r \, \mathrm{d}r \, \mathrm{d}\theta, \tag{29}$$

where r_{c} is the dislocation loop core radius. With the equation $\sigma^{1}_{zz} = \sigma^{\infty}_{zz} + \sigma^{\mathrm{v}}_{zz}$, after substitution of equations (4) and (13) into equation (29), we rewrite this formula as follows: $W^{1} = (1 - \tilde{r}_{\mathrm{c}})\pi^2 D b^2 R_0 q(\tilde{R}, \tilde{r}_{\mathrm{c}})$. Here $\tilde{r}_{\mathrm{c}} = r_{\mathrm{c}}/R_0$, $b = |b_z|$ is the MD loop

Burgers vector magnitude, $D = G/2\pi(1-\nu)$ and

$$q(\tilde{R}, \tilde{r}_c) = J(1,1;0)\big|_{\substack{\tilde{r}=1-\tilde{r}_c\\ \tilde{z}=0}} - \int_0^\infty \left(\frac{\rho_1(k) - 2(2-\nu)\rho_2(k)}{k} I_1[k(1-\tilde{r}_c)] - (1-\tilde{r}_c) I_2[k(1-\tilde{r}_c)]\rho_2(k) \right) k^3 \mathrm{d}k. \quad (30)$$

The first and second terms on the right-hand side of equation (30) correspond to the proper energy of the MD loop in an infinite medium and the difference between the proper energy MD of loops located in a cylinder and an infinite medium. In order to estimate the value of integral $J(1,1;0)|_{\substack{\tilde{r}=1-\tilde{r}_c\\ \tilde{z}=0}}$ in equation (30), it is convenient to use its asymptotic representation at $\tilde{r}_c \ll 1$ (for details, see Dundurs and Salamon (1972)): $J(1,1;0)|_{\substack{\tilde{r}=1-\tilde{r}_c\\ \tilde{z}=0}} \approx (1/\pi)[\ln(8/\tilde{r}_c) - 2]$.

The energy $W^{\mathrm{l-f}}$ that characterizes the interaction between the MD loop and the misfit stresses is calculated using the general formula (Mura 1968):

$$W^{\mathrm{l-f}} = b_z \int_0^{2\pi} \int_0^{R_0} \sigma_{zz}^{\mathrm{f}} r \, \mathrm{d}r \, \mathrm{d}\theta, \quad (31)$$

where σ_{zz}^{f} is the zz component of the misfit stress field, calculated by the formula (Gutkin *et al.* 2000)

$$\sigma_{zz}^{\mathrm{f}} = 2Gf \frac{1+\nu}{1-\nu} \left(\frac{\nu R_0^2 - R^2}{R^2} \Theta(R_0 - r) + \frac{\nu R_0^2}{r^2} \Theta(r - R_0) \right). \quad (32)$$

(Note that the formula for σ_{zz}^{f} in the paper by Gutkin *et al.* (2000) contains a misprint corrected here.) Here $\Theta(t)$ is the Heaviside function, equal to 1, for $t > 0$, and to 0, for $t < 0$. With equation (32) substituted into equation (31), we obtain

$$W^{\mathrm{l-f}} = -4\pi^2(1+\nu) D b_z R_0^2 f \left(1 - \frac{\nu}{\tilde{R}^2} \right). \quad (33)$$

The energy W^{c} of the dislocation loop core is given by the approximate formula (Hirth and Lothe 1982) $W^{\mathrm{c}} \approx (Db^2/2)l$. Here $l = 2\pi R_0$ is the length of the MD loop.

With the formulae for W^{l}, $W^{\mathrm{l-f}}$ and W^{c} substituted into equation (1) for ΔW, we find the following condition for the formation of the MD loop in a composite nanowire to be energetically favourable: $|f| > f_{\mathrm{c}}$, where

$$f_{\mathrm{c}} = \frac{\pi(1-\tilde{r}_c) q(\tilde{R}, \tilde{r}_c) + 1}{4\pi(1+\nu)(R_0/b)\left(1 - \nu/\tilde{R}^2\right)}. \quad (34)$$

f_{c} given by equation (34) represents the critical misfit parameter for the energetically favourable formation of the MD loop with $b_z = +b$ (if $f > 0$) or $b_z = -b$ (if $f < 0$).

The dependences of the critical misfit parameter f_{c} on the film thickness h are shown in figure 6 (a), for $\nu = 0.3$, $r_{\mathrm{c}} = b$ and different values of R_0. For comparison, the dependences of the critical misfit parameter $f_{\mathrm{c}}^{\mathrm{d}}$ for the formation of straight misfit dislocations (calculated by Gutkin *et al.* (2000)) are shown, too. For clarity, curve 1 in figure 6 (a) is also presented in figure 6 (b) on a larger scale. The broken line in figure 6 (b) shows the critical misfit parameter f_{c}^{∞} that corresponds to the case when $h \to \infty$, in which the two-phase composite cylinder transforms into a cylindrical inclusion in an infinite medium. As follows from figure 6, the dependences $f_{\mathrm{c}}(h)$

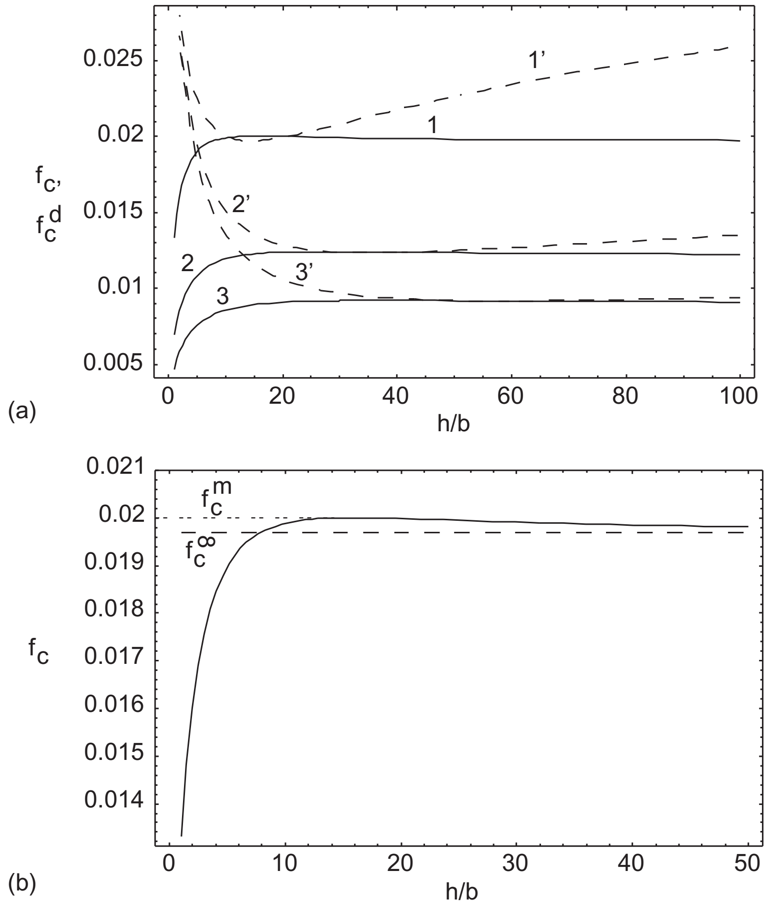


Figure 6. Dependences of critical misfit parameters f_c and f_c^d on non-dimensional film thickness h/b, for $\nu = 0.3$ and $r_c = b$. (a) the case when $R_0/b = 10$, 20 and 30, with dependences $f_c(h/b)$ shown as solid curves 1, 2 and 3, respectively, and dependences $f_c^d(h/b)$ shown as broken curves 1′, 2′ and 3′, respectively; (b) the case when $R_0/b = 10$, where the broken line shows the misfit parameter f_c^∞.

have maximums $f_c = f_c^m$ when the film thickness becomes larger by a small value than the substrate radius. (The maximums are weakly distinguished in figure 6 (a), because curves $f_c(h)$ weakly fall in the regions to the right of their maxima. However, they are well distinguished, if the scale of figure changes; see, for example figure 6 (b).) For $f_c > f_c^m$, the formation of the MD loop is energetically favourable at any value of the film thickness h (at a fixed value of the substrate radius R_0). If $f_c^\infty < f < f_c^m$, the formation of the MD loop can occur in a certain range of values of film thickness h. In the situation with $f < f_c^\infty$, the MD loop can be formed, if the film thickness h is lower than some critical thickness. Thus, the conditions for the energetically favourable formation of a MD loop in a two-phase composite cylinder (nanowire) are significantly different from those of the formation of a straight MD in such a cylinder. The formation of a straight MD is energetically favourable, if film and substrate thicknesses are close to each other, and only at sufficiently large values of f and R_0 (see figure 6 (a)). As follows from figure 6 (a), at identical values of f and R_0, the critical misfit parameter f_c for the formation of MD loops is commonly lower

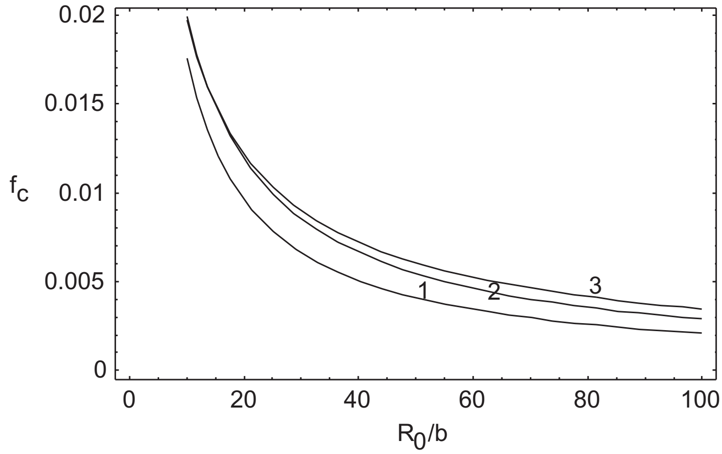


Figure 7. Critical misfit parameter f_c as a function of non-dimensional substrate radius R_0/b, for $\nu = 0.3$, $r_c = b$ and $h/b = 3$ (curve 1) $h/b = 10$ (curve 2) and $h/b = \infty$ (curve 3).

than the critical misfit parameter f_c^d for the energetically favourable formation of straight MDs ($f_c < f_c^d$). There is just one exception from the above statement. In small intervals of h, where $h \approx R_0$ (or h is larger than R_0 by a small value) and the curves $f_c(h)$ have their maxima, while the curves $f_c^d(h)$ have their minima, we have $f_c > f_c^d$. Thus, in wide ranges of the geometric parameters R_0 and h of a two-phase nanowire, the formation of MD loops (figure 1) may occur at smaller misfit values than the formation of straight MDs.

The dependences $f_c(R_0)$ are presented in figure 7, for $\nu = 0.3$, $r_c = b$ and various values of the film thickness h. As follows from figure 7, f_c decreases with rising R_0 (see also figure 6 (a)), approaching zero in the limit which $R_0 \to \infty$. For $h > 10b$, f_c is very close to the critical value f_c^∞ of misfit parameter for a cylindrical second-phase inclusion in an infinite medium (see curves 2 and 3 in figure 7). However, for very thin films with a thickness of several atomic layers, $f_c(h)$ is essentially lower than f_c^∞ (see curves 1 and 3 in figure 7).

§ 5. Concluding remarks

Thus, in this paper, we have suggested and theoretically examined a new relaxation mechanism in strained composite nanowires, namely the formation of MD loops (figures 1, 2, 3 and 4). According to our theoretical analysis, MD loops may form at smaller misfit values than straight MDs in wide ranges of geometric characteristics of two-phase nanowires. Generally speaking, the formation of MD loops in composite nanowires is either desirable or disappointing, from an applications viewpoint, depending on the roles of composite nanowires in applications. So, the formation of MD loops in semiconducting composite nanowires, similar to MDs in quantum dots on substrates (for example Ovid'ko (2002) and Ovid'ko and Sheinerman (2002)), can lead to degradation of functional properties of nanowires. However, if the internal cylindrical region of a two-phase nanowire has a polyatomic composition sensitive to the stress field distribution in this internal cylinder, stress fields of MD loops are capable of causing a modulation of the chemical composition in the nanowire (figure 8). Such composite nanowires have the potential to be exploited in nanotechnologies related to data storage and information processing

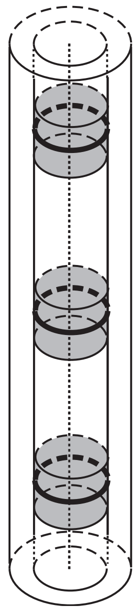


Figure 8. Modulation of chemical composition in internal cylindrical region of nanowire, induced by stress fields of MD loops (schematically).

(Lauhon *et al.* 2002). In the context discussed, experimental identification of MD loops in two-phase nanowires, being MD configurations of a new type will be of special importance.

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APPENDIX A

This appendix deals with calculation of Fourier images $\hat{\sigma}_{rr}^{\infty}(\tilde{R}, k)$ and $\hat{\sigma}_{rz}^{\infty}(\tilde{R}, k)$ of the stresses $\sigma_{rr}^{\infty}(\tilde{R}, \tilde{z})$ and $\sigma_{rz}^{\infty}(\tilde{R}, \tilde{z})$ respectively in equations (26) and (27). These Fourier images are calculated with the help of equations (2) and (5) as follows:

$$\hat{\sigma}_{rr}^{\infty}(\tilde{R}, k) = -M\left(\frac{1-2\nu}{\tilde{R}}\hat{J}(1,1;0) + F\Big[|\tilde{z}|J(1,0;2)\Big] - \hat{J}(1,0;1) - \frac{1}{\tilde{R}}F\Big[|\tilde{z}|J(1,1;1)\Big]\right)\Bigg|_{\tilde{r}=\tilde{R}}, \tag{A 1}$$

$$\hat{\sigma}_{rz}^{\infty}(\tilde{R}, k) = MF\Big[\tilde{z}J(1,1;2)\Big]\Big|_{\tilde{r}=\tilde{R}}. \tag{A 2}$$

For calculation of $\hat{\sigma}_{rr}^{\infty}(\tilde{R},k)$ and $\hat{\sigma}_{rz}^{\infty}(\tilde{R},k)$, let us find expressions for $\hat{J}(1,1;0)$, $\hat{J}(1,0;1)$, $F[|\tilde{z}|J(1,0;2)]$, $F[|\tilde{z}|J(1,1;1)]$ and $F[\tilde{z}J(1,1;2)]$ appearing in equations (A 1) and (A 2). To do this, let us consider the double integral $\hat{J}(m,n;p) = \int_{-\infty}^{\infty}\int_0^{\infty} J_m(t)J_n(\tilde{r}t)\exp(-|\tilde{z}|t)t^p \mathrm{d}t \exp(-\mathrm{i}k\tilde{z})\,\mathrm{d}\tilde{z}$. A change in the integration order and single integration (with respect to $\tilde{z}$) in this integral allows us to represent it in the following form:

$$\hat{J}(m,n;p) = 2\int_0^{\infty} \frac{J_m(t)J_n(\tilde{r}t)t^{p+1}}{t^2+k^2}\,\mathrm{d}t. \tag{A 3}$$

Using the same operations, the double integrals

$$F\Big[|\tilde{z}|J(m,n;p)\Big] = \int_{-\infty}^{\infty}\int_0^{\infty} J_m(t)J_n(\tilde{r}t)\exp(-|\tilde{z}|t)t^p\mathrm{d}t\ |\tilde{z}|\exp(-\mathrm{i}k\tilde{z})\,\mathrm{d}\tilde{z}$$

and

$$F\Big[\tilde{z}J(m,n;p)\Big] = \int_{-\infty}^{\infty}\int_0^{\infty} J_m(t)J_n(\tilde{r}t)\exp(-|\tilde{z}|t)t^p\mathrm{d}t\ \tilde{z}\exp(-\mathrm{i}k\tilde{z})\,\mathrm{d}\tilde{z}$$

can be written as follows:

$$F\Big[|\tilde{z}|J(m,n;p)\Big] = 2\int_0^{\infty} J_m(t)J_n(\tilde{r}t)\frac{t^p(t^2-k^2)}{(t^2+k^2)^2}\,\mathrm{d}t, \tag{A 4}$$

$$F\Big[\tilde{z}J(m,n;p)\Big] = -4\mathrm{i}k\int_0^{\infty} \frac{J_m(t)J_n(\tilde{r}t)t^{p+1}}{(t^2+k^2)^2}\,\mathrm{d}t. \tag{A 5}$$

With the right-hand sides of equations (A 4) and (A 5) compared with that of equation (A 3), we find that

$$F\Big[|\tilde{z}|J(m,n;p)\Big] = \hat{J}(m,n;p-1) + |k|\frac{\partial \hat{J}(m,n;p-1)}{\partial |k|}\ , \tag{A 6}$$

$$F\Big[\tilde{z}J(m,n;p)\Big] = \mathrm{i}\frac{\partial \hat{J}(m,n;p)}{\partial k}. \tag{A 7}$$

In order to calculate the integrals $\hat{J}(m,n;p)|_{\tilde{r}=\tilde{R}}$, we shall use the following relationship (Ditkin and Prudnikov 1974):

$$\int_0^{\infty} \frac{J_m(t)J_n(\tilde{r}t)t^{m-n+1}}{t^2+k^2}\,\mathrm{d}t = |k|^{n-m}I_m(|k|)K_n(\tilde{r}|k|), \quad \tilde{r} > 1, 1+n \geqslant m > -1. \tag{A 8}$$

In the considered situation with the MD loop in a composite cylinder (nanowire), we have $\tilde{R} > 1$. In these circumstances, substitution of equation (A 8) into equation (A 3), for $m = n = 1$ and $p = 0$, yields

$$\hat{J}(1,1;0)|_{\tilde{r}=\tilde{R}} = 2I_1(|k|)K_1(\tilde{R}|k|). \tag{A 9}$$

In order to calculate integral $\hat{J}(1,0;1)|_{\tilde{r}=\tilde{R}}$, let us represent it, using equation (A 3), in the following form:

$$\hat{J}(1,0;1)|_{\tilde{r}=\tilde{R}} = 2\int_0^{\infty} \frac{J_1(t)J_0(\tilde{R}t)t^2}{t^2+k^2}\,\mathrm{d}t. \tag{A 10}$$

Also, we shall use the relationship

$$\int_0^\infty J_1(t)J_0(\tilde{R}t)\,\mathrm{d}t = 0, \quad \tilde{R} > 1. \tag{A 11}$$

With the equation $t^2/(t^2+k^2) = 1 - k^2/(t^2+k^2)$ substituted into equation (A 10), and equation (A 11) taken into account, we obtain

$$\hat{J}(1,0;\,1)|_{\tilde{r}=\tilde{R}} = -2k^2\int_0^\infty \frac{J_1(t)J_0(\tilde{R}t)}{t^2+k^2}\mathrm{d}t = -2|k|I_1(|k|)K_0(\tilde{R}|k|). \tag{A 12}$$

Integral $\hat{J}(1,1;\,2)$, in its turn, can be represented with the help of equation (A 8) and the equation $t^3/(t^2+k^2) = t - k^2t/(t^2+k^2)$ in the following form:

$$\hat{J}(1,1;\,2)|_{\tilde{r}=\tilde{R}} = 2\left(\int_0^\infty J_1(t)J_1(\tilde{R}t)t\,\mathrm{d}t - k^2\int_0^\infty \frac{J_1(t)J_1(\tilde{R}t)t}{t^2+k^2}\mathrm{d}t\right). \tag{A 13}$$

From equations (A 8) and (A 13), one finds that

$$\left.\frac{\partial \hat{J}(1,1;\,2)}{\partial k}\right|_{\tilde{r}=\tilde{R}} = -2\frac{\partial}{\partial k}\big(k^2I_1(|k|)K_1(\tilde{R}|k|)\big). \tag{A 14}$$

Substitution of equation (A 12) into equation (A 6) with $m=1$, $n=0$, and $p=2$, insertion of equation (A 9) into equation (A 6) with $m=n=p=1$, and substitution of equation (A 14) into equation (A 7) with $m=n=1$ and $p=2$ yield

$$F[|\tilde{z}|J(1,0;\,2)]|_{\tilde{r}=\tilde{R}} = -2|k|\big\{I_1(|k|)\big[K_0(\tilde{R}|k|) - \tilde{R}|k|K_1(\tilde{R}|k|)\big] + |k|I_0(|k|)K_0(\tilde{R}|k|)\big\}, \tag{A 15}$$

$$F[|\tilde{z}|J(1,1;\,1)]|_{\tilde{r}=\tilde{R}} = 2|k|\big\{-\tilde{R}I_1(|k|)K_0(\tilde{R}|k|) + I_0(|k|)K_1(\tilde{R}|k|)\big\}, \tag{A 16}$$

$$F[\tilde{z}J(1,1;\,2)]|_{\tilde{r}=\tilde{R}} = \mathrm{i}kF[|\tilde{z}|J(1,1;\,1)]|_{\tilde{r}=\tilde{R}}. \tag{A 17}$$

In deriving equations (A 15)–(A 17), the recurrent relationships $I_1'(x) = I_0(x) - I_1(x)/x$, $K_0'(x) = -K_1(x)$, $K_1'(x) = -[K_0(x)+K_2(x)]/2$ and $K_2(x) = K_0(x) + (2/x)K_1(x)$ between the modified Bessel functions have been used.

With equations (A9), (A 12) and (A 15)–(A 17) substituted into equations (A 1) and (A 2), we find the following expressions for $\hat{\sigma}_{rr}^{\infty}(\tilde{R},k)$ and $\hat{\sigma}_{rz}^{\infty}(\tilde{R},k)$:

$$\begin{aligned}\hat{\sigma}_{rr}^{\infty}(\tilde{R},k) = -2M|k|\Bigg\{&I_1(|k|)\left[\left(\tilde{R}|k| + \frac{2(1-\nu)}{\tilde{R}|k|}\right)K_1(\tilde{R}|k|) + K_0(\tilde{R}|k|)\right]\\ &- |k|I_0(|k|)\left(K_0(\tilde{R}|k|) + \frac{K_1(\tilde{R}|k|)}{\tilde{R}|k|}\right)\Bigg\},\end{aligned} \tag{A 18}$$

$$\hat{\sigma}_{rz}^{\infty}(\tilde{R},k) = 2M\mathrm{i}k^2\,\mathrm{sgn}\,k\,\big[\tilde{R}I_1(|k|)K_0(\tilde{R}|k|) - I_0(|k|)K_1(\tilde{R}|k|)\big]. \tag{A 19}$$

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