Misfit stresses in a composite core-shell nanowire with an eccentric parallelepipedal core subjected to one-dimensional cross dilatation eigenstrain

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Abstract. The boundary-value problem in the classical theory of elasticity for a core-shell nanowire with an eccentric parallelepiped core of an arbitrary rectangular cross section is solved. The core is subjected to one-dimensional cross dilatation eigenstrain. The misfit stresses are given in a closed analytical form suitable for theoretical modeling of misfit accommodation in relevant heterostructures.

1. Motivation

Fabrication and studies of composite nanowires (NWs) is a necessary step in the development of modern nanotechnologies [1–4]. The difference in the crystal lattice parameters and thermal expansion coefficients of materials composing the NWs, causes the misfit strains and stresses in them. The physical characteristics of the NWs are strongly dependent on the level of misfit strains and stresses [5, 6]. On the other hand, it is well known that the misfit strains and stresses can relax through generation of various defects, in particular, misfit dislocations [7–10]. Theoretical models of defect formation in NWs were briefly reviewed in our recent work [11], where we developed an effective tool for theoretical modeling of misfit stress relaxation through dislocation glide along flat faces of parallelepipedal cores in core-shell NWs. This tool is a strict closed-form solution for stress fields in a core-shell NW, in which the core has a square cross section and occupies the symmetric position in the NW center. In work [11], the stress fields are caused by three-dimensional dilatation eigenstrain (3D misfit strain) and represented in the form of trigonometric series. Earlier, the stress fields in a similar core-shell NW were analyzed in the plane-strain case by the method of complex functions and visualized by maps of Cartesian stress components [12]. However, the satisfaction of boundary conditions was not proven. Moreover, the plane-strain state is not relevant for real core-shell NWs with three-dimensional mismatch of core and shell lattices.

Both the solutions found in [11] and [12] are restricted by the assumptions that the cores have square cross sections with their centers at the NW axes and are subjected to isotropic lattice misfit. In reality, the cores may have rectangular cross sections placed asymmetrically with respect to the NW axes, and the lattice misfit may be anisotropic due to the contact of materials with crystalline lattices of different types. This has motivated us to extend our recent solution [11] to the case of a core-shell...
NW with an eccentric parallelepipedal core of an arbitrary rectangular cross section, which is characterized by a one-dimensional (1D) cross dilatation eigenstrain with respect to the shell material. In the present work, we solve the corresponding boundary-value problem in the theory of elasticity and find its solution in a closed analytical form. Using numerical calculations, we illustrate our solution by the stress maps which prove the satisfaction of boundary conditions of the problem and show some interesting features in the stress distribution over the NW cross section.

2. Model

Our model is a long elastic cylinder containing an eccentric inclusion (core) in the form of a long parallelepiped with an arbitrary rectangular cross section (figure 1), in contrast with the special case in [11], where a symmetric core with a square cross section was considered. Both the cylinder and core are elastically homogeneous and isotropic and have identical elastic moduli: the shear modulus $G$ and the Poisson ratio $\nu$. The outer radius of the cylinder is $R$. The cross section of the core is a rectangle given by the coordinates of his vertexes. The core is subjected to a 1D dilatation eigenstrain $\varepsilon^*_{yy}$, in contrast with the case of isotropic 3D dilatation eigenstrain in [11]. It allows us to take into account the misfit-strain anisotropy in real composite NWs.

The stress field in such a composite cylinder $\sigma^{(y)}_y$ can be given by the sum of a stress field $\sigma^{(y)}_y$ caused by the core in an infinite body, and an extra stress field $\sigma^{(y)}_y$ which is required to fulfill the boundary conditions on the cylinder free surface:

$$\sigma^{cil}(y) = \sigma^{(y)}_y + \sigma^{(y)}_y.$$

The boundary conditions read

$$\sigma^{cil}(y)(r = R) = 0 \quad \text{and} \quad \sigma^{cil}(y)(r = R) = 0.$$

The non-vanishing stress components $\sigma^{(y)}_y$ are determined by the formulas [13]:

$$\sigma^{(y)}_y = C \psi^{(y)}_{xy} \bigg|_{x_1 = x_2} \bigg|_{y_1 = y_2}^0,$$

where $C = \varepsilon^*_{yy} G / [2\pi(1-\nu)]$ and

$$\psi^{(y)}_{xy} = \frac{(x-x_0)(y-y_0)}{(x-x_0)^2 + (y-y_0)^2}; \quad \psi^{(y)}_{xx} = \frac{(x-x_0)(y-y_0)}{(x-x_0)^2 + (y-y_0)^2} + 2\arctan \frac{y-y_0}{x-x_0};$$

$$\psi^{(y)}_{yy} = -\frac{(x-x_0)^2}{(x-x_0)^2 + (y-y_0)^2} - \ln \sqrt{(x-x_0)^2 + (y-y_0)^2}; \quad \psi^{(y)}_{yy} = 2\nu \arctan \frac{y-y_0}{x-x_0}.$$
Any stress function $\Psi_y$ in the cylindrical and Cartesian coordinate system can be calculated through the complex potentials [14] as

$$\Psi_{rr} + \Psi_{r\phi} = \Psi_{xx} + \Psi_{yy} = 2[F'(\zeta) + F(\zeta)] = 4\Re F'(\zeta),$$  \hspace{1cm} (5)

$$\Psi_{r\phi} - 2i\Psi_{r\phi} = [\Psi_{yy} - \Psi_{xx} + 2i\Psi_{xy}] e^{2i\phi} = 2[\overline{F}(\zeta) + \chi'(\zeta)] e^{2i\phi},$$ \hspace{1cm} (6)

where $F'(\zeta)$ and $\chi'(\zeta)$ are the complex potentials that are unknown analytical functions of the complex variable $\zeta = x + iy = re^{i\phi}$, $i = \sqrt{-1}$. $\overline{F(\zeta)}$ and $\overline{\chi(\zeta)}$ are the functions conjugate to $F'(\zeta)$ and $\chi'(\zeta)$, respectively.

Subtracting equations (5) from (6), we obtain the following formula which is convenient for the fulfillment of the boundary conditions:

$$\Psi_{rr} - i\Psi_{r\phi} = 1/2[[\Psi_{xx} + \Psi_{yy}] - [\Psi_{yy} - \Psi_{xx} + 2i\Psi_{xy}] e^{2i\phi}] = F'(\zeta) + \overline{F(\zeta)} - [\overline{F}(\zeta) + \chi'(\zeta)] e^{2i\phi},$$ \hspace{1cm} (7)

With taking into account the stress finiteness at $r \to 0$, we will search the functions $F'(\zeta)$ and $\chi'(\zeta)$ in the form of power series

$$F'(\zeta) = \sum_{n=0}^{\infty} A_n \zeta^n, \hspace{1cm} \chi'(\zeta) = \sum_{n=0}^{\infty} B_n \zeta^n,$$ \hspace{1cm} (8)

where $A_n$ and $B_n$ are complex constants in the general case. Now we could rewrite equation (7) as

$$\Psi_{rr} + i\Psi_{r\phi} = A_0 + \frac{A_0}{\zeta} + \sum_{n=1}^{\infty} \left[\sum_{n=1}^{\infty} \frac{1}{n-1} A_n + \frac{1}{R^2} B_{n-2}\right] \zeta^n.$$  \hspace{1cm} (9)

Let us find now the extra stress field $\sigma_{xy}^{(\gamma)}$ in the same form as that given by equation (3):

$$\sigma_{xy}^{(\gamma)} = C \Psi_{xy}^{(\gamma)} \left|_{x=x_0}^{x=x_1} \right| \left|_{y=y_0}^{y=y_1} \right.$$ \hspace{1cm} (10)

The boundary conditions (2) with account for equation (7) are

$$[[\Psi_{rr} + i\Psi_{r\phi}]_{R=R} = -1/2 \left[\Psi_{xx} + \bar{\Psi}_{yy} - \bar{\Psi}_{yy} - \Psi_{xx} + 2i\Psi_{xy}] e^{2i\phi}\right]_{R=R}.$$ \hspace{1cm} (11)

Let us introduce the new complex variables $\xi = Re^{i\phi}$, $\alpha = x_0 + iy_0$ and consider the terms in (11) separately:

$$\bar{\Psi}_{xx} + \bar{\Psi}_{yy} = 2 \arctan \frac{y_0 - y_0}{x - x_0} = 2 \arg(\xi - \alpha),$$ \hspace{1cm} (12)

$$-\bar{\Psi}_{yy} + 2i\Psi_{xy} e^{2i\phi} = -i \left[1 + \frac{\bar{\alpha} - \alpha}{\xi - \alpha} + 2 \ln(\xi - \alpha)\right] \frac{\xi^2}{R^2}. $$ \hspace{1cm} (13)

To satisfy the boundary conditions (2), we should represent equations (12) and (13) in terms of the power series. Finally, equation (11) reads

$$[[\Psi_{rr} + i\Psi_{r\phi}]_{R=R} = -\frac{1}{2} \sum_{n=1}^{\infty} \left[\frac{1}{n} - \frac{2 \alpha^2}{n + 2 R^2}\right] \left[\frac{\alpha}{\xi} - \frac{\alpha^2 + \alpha \bar{\alpha}}{\xi^2} - \sum_{n=2}^{\infty} \frac{1}{n} \left(\frac{\overline{\alpha \xi}}{R^2}\right)^n\right].$$ \hspace{1cm} (14)

Comparing the coefficients at $\xi^n$ in both equations (9) and (14), we have
The distribution of stress components \(\sigma_{rr}^{(y)}, \sigma_{\varphi\varphi}^{(y)}, \sigma_{\varphi\varphi}^{(z)}\) and \(\sigma_{\varphi z}^{(y)}\) in a cross section of the core-shell NW is shown in figure 2(a)–(d). It is evident that the \(\sigma_{rr}^{(y)}\) and \(\sigma_{\varphi\varphi}^{(y)}\) components satisfy the boundary conditions (2).
As is seen from figure 2, the stress fields are very inhomogeneous over the cross section of the NW and strongly screened by its free surface. The stresses $\sigma_r^{(y)}$ and $\sigma_r^{(\phi)}$ are concentrated near the edges of the core, while the stresses $\sigma_{pp}^{(y)}$ and $\sigma_{zz}^{(y)}$ show a rather unpredictable behavior. In fact, they are concentrated both at the “vertical” faces of the core and on the shell surface, at points

Figure 2. Distribution of the misfit stress components caused by the $\varepsilon_{yy}^*$ eigenstrain in the cross section of the core-shell NW: (a) $\sigma_r^{(y)}$, (b) $\sigma_r^{(\phi)}$, (c) $\sigma_{pp}^{(y)}$ and (d) $\sigma_{zz}^{(y)}$. The core position is defined by the coordinates of its vertices: $x_{1,2} = \pm 0.5R$, $y_1 = -0.2R$, $y_2 = 0.6R$. The stress values are given in units of $C = -\varepsilon_{yy}^* G /[2\pi(1-\nu)]$.
(±0.5, 0.9) for \(\tau_{pp}^{\text{cyl}}\), and (0, ±1) for both \(\tau_{pp}^{\text{cyl}}\) and \(\tau_{zz}^{\text{cyl}}\). It is also seen that the stress level can be rather high. For example, for typical values of \(|\varepsilon_{yy}| = 0.01\) and \(\nu = 0.3\), the \(C\) constant is of about \(G/440\) and, therefore, the stresses \(\tau_{rr}^{\text{cyl}}\) and \(\tau_{sp}^{\text{cyl}}\) reach the magnitude of about \((3.5 - 4)C = G/126 - G/110\), the stress \(\tau_{rr}^{\text{cyl}}\) reaches the magnitude of about \(C = G/440\), and the stress \(\tau_{zz}^{\text{cyl}}\) reaches the magnitude of about \(1.5C = G/293\). In metallic NWs, this stress level is quite enough for the onset of plastic relaxation processes even at room temperature, while in semiconductor NWs, it occurs under higher temperatures. The relaxation processes are expected to start either on the core-shell interface or on the shell surface.

4. Conclusions

In this paper, we have obtained a closed-form analytical solution for misfit stresses in a core-shell NW with an eccentric parallelepipedal core which is subjected to a 1D dilatation eigenstrain. It is shown that the solution satisfies the boundary conditions of the problem and gives a clear insight on the stress distribution in the NW. The stress fields are very inhomogeneous over the cross section of the NW and strongly screened by its free surface. Some stress components are concentrated at the edges of the core, while the others are concentrated at the core faces and on the shell surface. The stress magnitude can be sufficient for the onset of plastic relaxation processes in the NW under suitable temperature either on the core-shell interface or on the shell surface. We expect that our solution will be widely used in the theoretical description of the mechanisms for misfit accommodation in such NWs.

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