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. We present an analytical solution to the boundary-value problem in the classical theory of elasticity for a core-shell nanowire with an eccentric parallelepipedal core of an arbitrary rectangular cross section. The core is subjected to one-dimensional cross dilatation eigenstrain. The misfit stresses are found in a concise and transparent closed form which is convenient for practical use in theoretical modeling of misfit relaxation processes.

1. Introduction

Fabrication and studies of composite nanowires (NWs) is a necessary step in the development of modern nanotechnologies in optoelectronics, nanoscale field effect transistors, storage and data transmission devices, neural device sensors, etc. [1–10]. Physical properties of composite NWs depend on the shape, size, chemical composition, and types of crystalline lattices of the NW components as well as on the presence of various defects in their structure. In particular, the shape can be tightly related with peculiarities in misfit stress distribution over the NWs and with the mechanisms of misfit stress relaxation in them. However, in theoretical description of these mechanisms, they commonly use the model of cylindrically symmetric core-shell NWs [11–26] as it is much simpler for analytical modeling. The problem is that this simple approach strictly limits the variety of relaxation mechanisms available for theoretical examination. For example, it excludes the glide of straight misfit dislocations along the flat areas of the core-shell interface that is sometimes observed in experiments [27, 28]. It is worth noting that flat interface regions often form in radially inhomogeneous NWs [29–32].

It seems that the simplest case of a core with flat faces is the core in the form of a long parallelepiped. To our best knowledge, today there are two analytical solutions which describe the elastically strained state in a core-shell NW with a square core placed symmetrically with respect to the shell surface [33, 34]. The solution [33] was found in the model case of plane strain through the complex potentials method and illustrated by stress maps in Cartesian coordinates. The drawback of the work [33] is that the authors did not demonstrate the evidence of the boundary condition fulfillment. Moreover, the case of plane strain is obviously quite far from the case of three-dimensional mismatch of crystalline lattices in real core-shell NWs. In work [34], the stress field
caused by dilatation eigenstrain (3D misfit strain), was found in the form of trigonometric series. However, the solution [34] does not allow to consider the case of dilatation anisotropy in composite NWs which consist of materials with different crystalline lattices.

The present work is aimed at the analytical calculation and numerical analysis of the misfit stresses in a core-shell NW with an eccentric parallelepiped core of an arbitrary rectangular cross section, which is characterized by a one-dimensional cross dilatation eigenstrain with respect to the shell material. We show the analytical formulas for the misfit stress components applicable for practical use in theoretical modeling of anisotropic misfit stress and relaxation processes. We also demonstrate some examples of stress distribution in the NW cross section, from which the fulfillment of boundary conditions on the shell free surface is evident.

2. Model

Consider a long core-shell cylinder of radius $R$, which consists of an elastically homogeneous and isotropic shell and a core having the shape of a long parallelepiped (figure 1). The shear modulus $G$ and the Poisson ratio $\nu$ are the same for the shell and the core. The core cross section is a rectangle given by the coordinates of his vertexes. The core is subjected to a dilatation eigenstrain $\varepsilon^{yy}$.

The desired stress field $\sigma_{ij}^{(y)}$ caused by the $\varepsilon^{yy}$ eigenstrain can be represented by the sum of a similar stress field $\sigma_{ij}^{(y)}$ created by the core in an infinite medium, and an extra stress field $\sigma_{ij}^{(s)}$ which is needed to satisfy the boundary conditions on the shell free surface:

$$\sigma_{ij}^{(y)} = \sigma_{ij}^{(y)} + \sigma_{ij}^{(s)}. \quad (1)$$

The boundary conditions are

$$\varepsilon_{rr}^{(y)}(r = R) = 0 \quad \text{and} \quad \varepsilon_{r\phi}^{(y)}(r = R) = 0. \quad (2)$$

The non-vanishing stress components $\sigma_{ij}^{(s)}$ are given as follows [35]:

$$\sigma_{ij}^{(s)} = C \Psi_{ij}^{(s)} \bigg|_{x=x_1}^{x=x_2} \bigg|_{y=y_1}^{y=y_2}, \quad (3)$$

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

$$\Psi_{xx}^{(s)} = \frac{(x-x_0)(y-y_0)}{(x-x_0)^2 + (y-y_0)^2}; \quad \Psi_{yy}^{(s)} = \frac{(x-x_0)(y-y_0)}{(x-x_0)^2 + (y-y_0)^2} + 2\arctan \frac{y-y_0}{x-x_0};$$

$$\Psi_{xy}^{(s)} = \Psi_{yx}^{(s)} = \frac{(x-x_0)^2}{(x-x_0)^2 + (y-y_0)^2} - \ln \sqrt{(x-x_0)^2 + (y-y_0)^2}; \quad \Psi_{zz}^{(s)} = 2\nu \arctan \frac{y-y_0}{x-x_0}. \quad (4)$$
Any stress function \( \Psi_{ij} \) in the cylindrical and Cartesian coordinate system can be calculated through the complex potentials [36] as

\[
\Psi_{rr} + \Psi_{\phi\phi} = \Psi_{xx} + \Psi_{yy} = 2[F'(\zeta) + F'(\bar{\zeta})] = 4 \Re F'(\zeta),
\]

\[
\Psi_{rr} - i \Psi_{\phi\phi} = [\Psi_{yy} - \Psi_{xx} + 2i \Psi_{xy} e^{2i\phi}] = 2[\overline{F'}(\zeta) + \chi'(\zeta)]e^{2i\phi},
\]

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

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

\[
\Psi_{rr} - i \Psi_{\phi\phi} = 1/2(\Psi_{xx} + \Psi_{yy} - \Psi_{xy} + 2i \Psi_{xy} e^{2i\phi}) = F'(\zeta) + F'(\bar{\zeta}) - 2F'(\zeta) - \chi'(\zeta) e^{2i\phi}. \quad (7)
\]

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

\[
F'(\zeta) = \sum_{n=0}^{\infty} A_n \zeta^n, \quad \chi'(\zeta) = \sum_{n=0}^{\infty} B_n \zeta^n, \quad (8)
\]

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

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

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

\[
\sigma_{ij}^{(y)} = C \Psi_{ij}^{(y)}(x, y), \quad (10)
\]

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

\[
[\Psi_{ij}^{(y)} - i \Psi_{\phi\phi}^{(y)}]_{R} = 1/2(\Psi_{ij}^{(y)} + \Psi_{ij}^{(y)} - \Psi_{ij}^{(y)} + 2i \Psi_{ij}^{(y)} e^{2i\phi})_{R} \quad (11)
\]

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

\[
- \Psi_{xx}^{(y)} - \Psi_{yy}^{(y)} = 2 \arctan \frac{y_0 - y}{x - x_0} = 2 \arg(\xi - \alpha), \quad (12)
\]

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

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

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

Comparing the coefficients at \( \zeta^n \) in both equations (9) and (14), we have

\[
A_0 = \frac{i}{2} \left( \frac{\alpha^2 + \alpha \bar{\alpha}}{R^2} \right), \quad A_n = \frac{i}{2} \left( R^2 - \alpha \bar{\alpha} \right) \frac{1}{n} \frac{2}{n + 2} \frac{\alpha^2}{R^2} \left( \frac{\alpha}{\bar{\xi}} \right)^n, \quad n = 1, 2, 3, \ldots
\]
\[ B_n = -\frac{i R^2}{2} \left[ \frac{\alpha \bar{\alpha} - 2 \bar{\alpha}^2}{R^2} + (n+2) \frac{R^2 - \alpha \bar{\alpha}}{R^2} + 2(n+1) \frac{\bar{\alpha}^2}{(n+4) R^2} \right] \left( \frac{\bar{\alpha}}{R^2} \right)^{n+2}, \quad n = 1,2,3... \] (15)

Substitution of equations (15) and (8) to (5), (6) gives the complex form for the stress function of the extra stress tensor:

\[ \Psi_{rr}^{(y)} + \Psi_{\bar{r}\bar{r}}^{(y)} = 2 x_0 y_0 \frac{R^2}{R^2} - 2 \operatorname{Im} \left\{ \frac{\alpha \bar{\alpha}}{R^2 - \bar{\alpha}^2} + \frac{2 R^2 - \bar{\alpha}^2}{\zeta^2} \ln \left( \frac{R^2 - \bar{\alpha}^2}{\zeta^2} \right) \right\}, \]

\[ \Psi_{r\bar{r}}^{(y)} + 2i \Psi_{\bar{r}r}^{(y)} = i \left\{ -\frac{\alpha \bar{\alpha}}{R^2} + \frac{2 R^2 - \bar{\alpha}^2}{R^2 - \bar{\alpha}^2} - \frac{\alpha \bar{\alpha} - r^2}{R^2 - \bar{\alpha}^2} \right\} - \frac{R^2 - r^2}{r^2} \left( \frac{\alpha \bar{\alpha}}{R^2 - \bar{\alpha}^2} \right)^2 \left( \frac{2 R^2 - \bar{\alpha}^2}{\zeta^2} \right) \ln \left( \frac{R^2 - \bar{\alpha}^2}{\zeta^2} \right). \] (16)

Transforming equations (16), we come to the final components of the extra stress tensor:

\[ \Psi_{rr}^{(y)} = -\frac{1}{2} \left\{ q^2 1 - \frac{1}{t^2} \left[ \sin 2 \theta + 2 \sin 2 \theta - q^2 t^2 \sin (\varphi + \theta) \right] + \frac{q(1 - q^2)(1 - t^2)(1 - q^2 t^2) \sin (\varphi - \theta)}{t \Lambda} + 2 \left[ P \cos 2 \varphi \arctan \Phi + \sin 2 \varphi \ln \sqrt{\Lambda} \right] \right\}; \]

\[ \Psi_{r\bar{r}}^{(y)} = -\frac{1}{2} \left\{ q^2 - \cos 2 \theta + 2 q 1 - \frac{1}{t^2} \cos 2 \theta - q^2 t^2 \cos (\varphi + \theta) \right\} + \frac{q(1 - q^2)(1 - t^2)(1 - q^2 t^2) \cos (\varphi - \theta)}{t \Lambda} + 2 \left[ \sin 2 \varphi \arctan \Phi - \cos 2 \varphi \ln \sqrt{\Lambda} \right]; \]

\[ \Psi_{\bar{r}r}^{(y)} = \frac{1}{2} \left\{ q^2 1 + \frac{1}{t^2} \left[ \sin 2 \theta - q^2 t^2 \sin (\varphi + \theta) \right] + \frac{q(1 - q^2)(1 - t^2)(1 - q^2 t^2) \sin (\varphi - \theta)}{t \Lambda} + 2 \left[ P \cos 2 \varphi - 1 \right] \arctan \Phi + P \sin 2 \varphi \ln \sqrt{\Lambda} \right\}; \]

\[ \Psi_{\bar{r}\bar{r}}^{(y)} = 2 \left\{ q^2 - 2 \theta - q^2 t^2 \sin (\varphi - \theta) + 2 \cos 2 \varphi - t^2 \arctan \Phi + \sin 2 \varphi \ln \sqrt{\Lambda} \right\}; \] (16)

where \( \rho \) and \( \theta \) are polar coordinates of the core vertex, and

\[ t = R / \rho; \quad a = \rho / R; \quad \Lambda = q^2 t^2 - 2qt \cos (\varphi - \theta) + 1; \quad \Phi = \frac{qt \sin (\varphi - \theta)}{1 - qt \cos (\varphi - \theta)}; \quad P = \frac{2t^2 + 3}{t^4}. \]

Thus, the problem under consideration (figure 1) is solved.

3. Results

To illustrate our solution, we show in figure 2(a)–(d) the distribution of stress components \( \sigma_{rr}^{(y)}, \sigma_{r\bar{r}}^{(y)}, \sigma_{\bar{r}r}^{(y)} \) and \( \sigma_{\bar{r}\bar{r}}^{(y)} \) in a cross section of the core-shell NW. It is evident that the \( \sigma_{rr}^{(y)} \) and \( \sigma_{r\bar{r}}^{(y)} \) components satisfy the boundary conditions (2).
4. Conclusions
We can conclude that our analytical solution, first, satisfies the boundary conditions of the problem, second, gives an opportunity to analyze the misfit stress distribution in detail, and, third, is represented in a concise and transparent closed form which is applicable for theoretical modeling of misfit stress relaxation processes.
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