Misfit stresses in a core-shell nanowire with core in the form of long parallelepiped

S A Krasnitckii1, A M Smirov2 and M Yu Gutkin1-3

1Peter the Great St. Petersburg Polytechnic University, 29 Polytekhnicheskaya str.,
St. Petersburg, 195251 Russia
2ITMO University, 49 Kronverkskii Ave., St. Petersburg, 197101 Russia
3Institute of Problems in Mechanical Engineering, Russian Academy of Sciences, 61
Bolshoi Ave., Vasil. Ostrov, St. Petersburg, 199178 Russia

Email: krasnitckii@gmail.com, smirnov.mech@gmail.com, m.y.gutkin@gmail.com

Abstract. We present an analytical solution to the boundary-value problem in the classical
theory of elasticity for a core-shell nanowire with a core in the form of a long parallelepiped
with a square cross section. The core is placed symmetrically with respect to the cylindrical
shell surface. The misfit stresses are found in a concise and transparent form of trigonometric
series, which is convenient for practical use in theoretical modeling of misfit relaxation
mechanisms. This work was supported by Peter the Great St. Petersburg Polytechnic
University and ITMO University.

1. Introduction
Radially inhomogeneous nanowires (NWs) demonstrate excellent electronic and optical properties,
which encourage their use in various devices of optoelectronics, nanoscale field effect transistors,
storage and data transmission devices, logic devices, sensors, etc. [1-10]. Physical properties of NWs
depend on the shape, size, chemical composition, and types of crystalline lattices of NW components
as well as on presence of various defects in their structure. In particular, the shape effects can be
tightly related with peculiarities in misfit stress distribution over 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 possible
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 with a square cross section. To our best knowledge, today there is only one analytical
solution which describes the elastically strained state in a core-shell NW with such a core placed
symmetrically with respect to the shell surface [33]. The solution was found in the model case of plane
strain through the complex potentials method and illustrated by stress maps in Cartesian coordinates.
The disadvantage 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.

The present work is aimed at the analytical calculation and numerical analysis of the misfit stresses in a core-shell NW with a symmetrically placed core which is characterized by a three-dimensional dilatation eigenstrain (3D misfit strain) with respect to the shell material and has the shape of a long parallelepiped with a square cross section. We show the analytical formulas for the misfit stress components applicable for practical use in theoretical modeling of misfit stress relaxation processes and demonstrate their 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 NW of radius $R$, which consists of 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 square with a side $2a$. The core is centered symmetrically with respect to the shell surface and subjected to the 3D homogeneous dilatation eigenstrain $\varepsilon^*$. The desired stress field $\sigma_{ij}$ caused by the eigenstrain $\varepsilon^*$ can be represented by the sum of a similar stress field $\sigma_{ij}^\infty$ created by the core in an infinite medium, and an extra stress field $\sigma_{ij}^*$ which is needed to satisfy the boundary conditions on the shell free surface:

$$\sigma_{ij} = \sigma_{ij}^\infty + \sigma_{ij}^*.$$  (1)

The boundary conditions are:

$$\sigma_{rr}^*(r = R) = -\sigma_{rr}^\infty(r = R); \quad \sigma_{r\theta}^*(r = R) = -\sigma_{r\theta}^\infty(r = R).$$  (2)

The non-vanishing stress components $\sigma_{ij}^\infty$ are given as follows [34]:

$$\sigma_{xx}^\infty = 2C \left[ \arctan \frac{x-a}{y+a} + \arctan \frac{x+a}{y-a} - \arctan \frac{x-a}{y+a} - \arctan \frac{x+a}{y-a} \right];$$  (3a)

$$\sigma_{xy}^\infty = 2C \ln \left[ \frac{(x-a)^2 + (y-a)^2}{[(x-a)^2 + (y+a)^2][(x+a)^2 + (y-a)^2]} \right];$$  (3b)

$$\sigma_{yy}^\infty = 2C \left[ \arctan \frac{y+a}{x-a} + \arctan \frac{y-a}{x+a} - \arctan \frac{y-a}{x+a} - \arctan \frac{y+a}{x-a} \right];$$  (3c)

$$\sigma_{zz}^\infty = \begin{cases} -4\pi C, & |x| \leq a, \ |y| \leq a \\ 0, & |x| > a, \ |y| > a \end{cases};$$  (3d)

Figure 1. Cross section of a core-shell nanowire of radius $R$ with a core in the form of a long parallelepiped with a square cross section $2a \times 2a$. 

The cross section of a core-shell nanowire of radius $R$ with a core in the form of a long parallelepiped with a square cross section $2a \times 2a$. 

The boundary conditions are:

$$\sigma_{rr}^*(r = R) = -\sigma_{rr}^\infty(r = R); \quad \sigma_{r\theta}^*(r = R) = -\sigma_{r\theta}^\infty(r = R).$$  (2)

The non-vanishing stress components $\sigma_{ij}^\infty$ are given as follows [34]:

$$\sigma_{xx}^\infty = 2C \left[ \arctan \frac{x-a}{y+a} + \arctan \frac{x+a}{y-a} - \arctan \frac{x-a}{y+a} - \arctan \frac{x+a}{y-a} \right];$$  (3a)

$$\sigma_{xy}^\infty = 2C \ln \left[ \frac{(x-a)^2 + (y-a)^2}{[(x-a)^2 + (y+a)^2][(x+a)^2 + (y-a)^2]} \right];$$  (3b)

$$\sigma_{yy}^\infty = 2C \left[ \arctan \frac{y+a}{x-a} + \arctan \frac{y-a}{x+a} - \arctan \frac{y-a}{x+a} - \arctan \frac{y+a}{x-a} \right];$$  (3c)

$$\sigma_{zz}^\infty = \begin{cases} -4\pi C, & |x| \leq a, \ |y| \leq a \\ 0, & |x| > a, \ |y| > a \end{cases};$$  (3d)
where \( C = G e^{- \nu / (1 + \nu)} / [2\pi (1 - \nu)] \).

To satisfy the boundary conditions (2), we should represent Eqs. (3a)-(3c) in the cylindrical coordinate system on the shell surface \( r = R \). First, let us consider the following derivative:

\[
\frac{d}{d\theta} \left( \arctan \frac{y + a}{x - a} \bigg|_{y = R \sin \theta, \ x = R \cos \theta} \right) = \frac{1 - \rho \cos(\theta + \pi/4)}{1 - 2 \rho \cos(\theta + \pi/4) + \rho^2},
\]

where \( \rho = \sqrt{2a / R}, \rho < 1 \). The r.h.s. of Eq. (4) can be expanded in a Fourier series [35] as

\[
\frac{1 - \rho \cos(\theta + \pi/4)}{1 - 2 \rho \cos(\theta + \pi/4) + \rho^2} = \sum_{n=0}^{\infty} \rho^n \cos(k(\theta + \pi/4)).
\]

Integrating series (5) over \( \theta \), we find the trigonometric series for the desired function:

\[
\arctan \frac{y + a}{x - a} = \Theta(\theta) + \sum_{n=1}^{\infty} \frac{1}{n} \rho^n \sin(k(\theta + \pi/4)),
\]

where \( \Theta(\theta) = \begin{cases} \theta, & \text{for } -\pi < \theta \leq -\arccosa / R \\ \arccosa / R < \theta \leq \arccosa / R, & \theta - \pi, \end{cases} \)

Applying the same procedure to every function figuring in Eqs. (3a)-(3c), after some algebra we find the following compact formulas for the stress fields \( \sigma_{yy}^* \) on the shell surface \( r = R \):

\[
\sigma_{yy}^*(r = R) = 4C \sum_{k=1}^{\infty} \frac{(-1)^k}{2k-1} \rho^{4k-2} \cos[(4k - 2)\theta];
\]

\[
\sigma_{yx}^*(r = R) = 4C \sum_{k=1}^{\infty} \frac{(-1)^k}{2k-1} \rho^{4k-2} \sin[(4k - 2)\theta];
\]

\[
\sigma_{xy}^*(r = R) = -4C \sum_{k=1}^{\infty} \frac{(-1)^k}{2k-1} \rho^{4k-2} \cos[(4k - 2)\theta].
\]

We can now rewrite the stress tensor \( \sigma_{yy}^* \) in the cylindrical coordinate system. Using the well-known formulas:

\[
\sigma_{\theta\theta}^* = \sigma_{xx}^* \cos^2 \theta + 2\sigma_{xy}^* \cos \theta \sin \theta + \sigma_{yy}^* \sin^2 \theta;
\]

\[
\sigma_{\theta\phi}^* = (\sigma_{yy}^* - \sigma_{xx}^*) \cos \theta \sin \theta + \sigma_{xy}^* (\cos^2 \theta - \sin^2 \theta);
\]

\[
\sigma_{\phi\phi}^* = \sigma_{xx}^* \sin^2 \theta - 2\sigma_{xy}^* \cos \theta \sin \theta + \sigma_{yy}^* \cos^2 \theta,
\]

with Eqs. (7) we come to the final formulas for the stress components \( \sigma_{yy}^* \) in the cylindrical coordinate system:

\[
\sigma_{\theta\phi}^*(r = R) = -4C \rho^2 \sum_{n=0}^{\infty} \frac{(-1)^n}{2n+1} (\rho)^{4n} \cos 4n\theta;
\]

\[
\sigma_{\phi\phi}^*(r = R) = 4C \rho^2 \sum_{n=0}^{\infty} \frac{(-1)^n}{2n+1} (\rho)^{4n} \cos 4n\theta.
\]

Let us now introduce the complex variable \( \xi = x + iy = re^{i\theta}, \ i = \sqrt{-1} \). The components of the extra stress tensor \( \sigma_{yy}^* \) in the cylindrical coordinate system can be calculated through the complex potentials [36] as:
\[
\sigma^*_r + \sigma^*_{\theta\theta} = 2[F'(\xi) + F''(\xi)];
\]

\[
\sigma^*_\theta - \sigma^*_r + 2i\sigma^*_{r\theta} = 2[i\bar{F}'(\xi) + \chi'(\xi)]e^{2i\theta},
\]

where \(F'(\xi)\) and \(\chi'(\xi)\) are the complex potentials that are unknown analytical functions of the complex variable \(\xi\), and \(F''(\xi)\) and \(\chi''(\xi)\) are the function conjugate with \(F'(\xi)\) and \(\chi'(\xi)\), respectively.

Subtracting Eq. (10b) from Eq. (10a), we obtain the following formula which is convenient for the fulfillment of the boundary conditions:

\[
\sum_{n=1}^{\infty} \sigma_n \xi^n, \quad \chi''(\xi) = \sum_{n=1}^{\infty} B_n \xi^n,
\]

where \(A_n\) and \(B_n\) are complex constants in the general case.

Substituting series (9a,b) and (11) into Eq. (10c) and taking into account that \(R \rightarrow 0\), we will search the functions \(F'(\xi)\) and \(\chi'(\xi)\) in the form of power series:

\[
F'(\xi) = \sum_{n=1}^{\infty} A_n \xi^n, \quad \chi'(\xi) = \sum_{n=1}^{\infty} B_n \xi^n,
\]

where \(A_n\) and \(B_n\) are complex constants in the general case.

Substituting series (9a,b) and (11) into Eq. (10c) and taking into account that \(r = R\) on the outer surface, after some algebra we find that:

\[
-4C \rho^2 \sum_{n=1}^{\infty} \left(\frac{1}{2n+1}\right) \rho^{4n} e^{-4i\theta} = A_0 + A_1 + \sum_{n=1}^{\infty} A_n R^{4n} e^{-4i\theta} - \sum_{n=1}^{\infty} (4n-1) A_n R^{4n} e^{-4i\theta} - \frac{1}{R} \sum_{n=1}^{\infty} B_n R^{4n} e^{-4i\theta}.
\]

Comparing the coefficients at \(e^{4i\theta}\) in both parts of this equation, we have:

\[
A_0 = A_0 = 2C \rho^2; \quad A_4 = A_{4n} = 4C \rho^2 \left(\frac{1}{2n+1}\right)^4 \rho^{4n}; \quad B_{4n-2} = -4C \rho^2 \left(\frac{1}{2n+1}\right) \rho^{4n}.
\]

Substitution of Eqs. (11) and (13) to Eqs. (10a,b) gives the final components of the extra stress tensor:

\[
\sigma^*_r = 4C \rho^2 \left[1 - \sum_{n=1}^{\infty} \left(\frac{1}{2n+1}\right)^4 \left(\frac{R}{r}\right)^2 \cos 4n\theta\right];
\]

\[
\sigma^*_\theta = 4C \rho^2 \left[\sum_{n=1}^{\infty} \left(\frac{1}{2n+1}\right)^4 \left(\frac{R}{r}\right)^2 \sin 4n\theta\right];
\]

\[
\sigma^*_{\theta\theta} = 4C \rho^2 \left[1 + \sum_{n=1}^{\infty} \left(\frac{1}{2n+1}\right)^4 \left(\frac{R}{r}\right)^2 \cos 4n\theta\right].
\]

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

3. Results

To illustrate our solution, we show in figures 2(a) and 2(b) the distribution of stress components \(\sigma^*_r, \sigma^*_\theta\), and \(\sigma^*_{r\theta}\) over the shell surface \(r = R\). It is evident that the \(\sigma^*_r\) and \(\sigma^*_\theta\) components satisfy the boundary conditions (2) with account for Eq. (1). Figures 2(c) and 2(d) demonstrate the maps of the stress components \(\sigma^*_{xy}\) and \(\sigma^*_{yx}\), respectively, in the cross section of the NW. As is seen, the shell free surface noticeably screens the misfit shear stress.
4. Conclusions
We can conclude that our analytical solution (1) satisfies the boundary conditions of the problem (2), gives an opportunity to analyze the misfit stress distribution in detail, and (3) is represented in a concise and transparent form which is applicable for theoretical modeling of misfit stress relaxation processes.

References
[1] Lauhon L J, Gudiksen M S and Lieber C M 2004 Phil. Trans. R. Soc. Lond. A 362 1247
[2] Mieszawska A J, Jalilian R, Sumanasekera G U and Zamborini F P 2007 Small 3 722
[3] Agarwal R 2008, Small 4 1872
[4] Comini E, Baratto C, Faglia G, Ferroni M, Vomiero A and Sberveglieri G 2009 Prog. Mater. Sci. 54 1
[5] Dubrovskii V G, Cirilin G E and Ustinov V M 2009 Semiconductors 43 1539
[6] Barth S, Hernandez-Ramirez F, Holmes J D and Romano-Rodriguez A 2010 Prog. Mater. Sci. 55 563
[7] Gao Q, Tan H H, Jackson H E, Smith L M, Yarrison-Rice J M, Zou J and Jagadish C 2011 Semicond. Sci. Technol. 26 014035
[8] Garnett E C, Brongersma M L, Cui Y and McGehee M D 2011 Annu. Rev. Mater. Res. 41 269
[9] Kenry C T 2013 Prog. Mater. Sci. 58 705
[10] Amato M, Palummo M, Rurai L and Ossicini S 2014 Chem. Rev. 114 1371
[11] Gutkin M Yu, Ovid'ko I A and Sheinerman A G 2000 J. Phys. Condens. Matter 12 5391
[12] Sheinerman A G and Gutkin M Yu 2001 Phys. Stat. Soli (A) 184 485
[13] Ovid'ko I A and Sheinerman A G 2004 Phil. Mag. 84 2103
[14] Liang Y, Nix W D, Griffin P B and Plummer J D 2005 J. Appl. Phys. 97 043519
[15] Raychaudhuri S and Yu E T 2006 J. Appl. Phys. 99 114308
[16] Aifantis K E, Kolesnikova A L and Romanov A E 2007 Phil. Mag. 87 4731
[17] Colin J 2010 Phys. Rev. B 82 054118
[18] Wang X, Pan E and Chung P W 2010 Int. J. Plasticity 26 1415
[19] Chu H J, Wang J, Zhou C Z and Beyerlein I J 2011 Acta Mater. 59 7114
[20] Gutkin M Yu, Kuzmin K V and Sheinerman A G 2011 Phys. Stat. Soli (B) 248 1651
[21] Haapamaki C M, Baugh J and LaPierre R R 2012 J. Appl. Phys. 112 124305
[22] Chu H J, Zhou C Z, Wang J and Beyerlein I J 2013 J. Mech. Phys. Solids 61 2147
[23] Dayeh S A, Tang W, Boioli F, Kavanagh K L, Zheng H, Wang J, Mack N H, Swadener G, Huang J Y, Miglio L, Tu K N and Picraux S T 2013 Nano Lett. 13 1869
[24] Salehzadeh O, Kavanagh K L and Watkins S P 2013 J. Appl. Phys. 114 054301
[25] Enzevaee C, Gutkin M Yu and Shodja H M 2014, Phil. Mag. 94 492
[26] Gutkin M Yu and Smirnov A M 2015 Acta Mater. 88 91
[27] Ding Y, Fan F, Tian Z and Wang Z L 2010, J. Am. Chem. Soc. 132 12480
[28] Bhattachari N, Casillas G, Ponce A and Jose-Yacaman M 2013 Surf. Sci. 609 161
[29] Wang Z L, Dai Z R, Gao R P, Bai Z G and Gole J L 2000 Appl. Phys. Lett. 77 3349
[30] Hu J, Bando Y, Liu Z, Sekiguchi T, Golberg D and Zhan J 2003 J. Am. Chem. Soc. 125 11306
[31] Teo B K, Li C P, Sun X H, Wong N B and Lee S T 2003 Inorg. Chem. 42 6723
[32] Qian F, Li Y, Gradečak S, Park H G, Dong Y, Ding Y, Wang Z L and Lieber C M 2008 Nature Materials 7 701
[33] Zou W-N, He Q-C and Zheng Q-S 2012 Int. J. Solids Struct. 49 1627
[34] Malyshkov K L, Gutkin M Yu, Romanov A E, Sitnikova A A and Sorokin L M 1988 Sov. Phys.-Solid State 30 1176
[35] Prudnikov A P Brychkov Yu A Marichev O I 1986 Integrals and Series 1 Elementary Functions Gordon & Breach Sci. Publ. (New York)
[36] Muskhelishvili N I 1977 Some Basic Problems of the Mathematical Theory of Elasticity Noordhoff Int. Publ. (Leyden, The Netherlands)