Misfit stress relaxation in composite core-shell nanowires with parallelepiped cores using rectangular prismatic dislocation loops

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Abstract. The misfit stress relaxation via generation of rectangular prismatic dislocation loops at the interface in core-shell nanowires is considered. The core has the shape of a long parallelepiped of a square cross-section. The energy change caused by loop generation in such nanowires is calculated. Critical conditions for the onset of such loops are calculated and analyzed.

1. Motivation
Thanks to their excellent physical properties, core-shell nanowires (NWs) are widely used in novel devices for optoelectronics, photonics, and spintronics [1-4]. The stability of physical properties depends on different structural and material factors including lattice mismatch, a difference in thermal coefficients of core and shell materials, and the presence of defects at the core/shell interfaces [5-10]. Currently, there are a number of theoretical models that describe how defects are generated, in particular, misfit dislocations [11-13]. The disadvantage of all these models is the assumption of axial symmetry of cores in core-shell NWs, although in reality the cores are shaped like polyhedral prisms with flat surfaces [14-16]. This approach does not allow to take into account the effects associated with the stress concentration at the edges of the interfaces. Moreover, it cannot be used in theoretical consideration of dislocations gliding along flat interfaces.

The simplest geometric model of an NW with flat core-shell interfaces is an elastic cylinder with a long parallelepiped inclusion. Recently, we have obtained a solution for the boundary value problem in the theory of elasticity for an elastic cylinder with an eccentric inclusion of a rectangular cross section subjected to a dilatation eigenstrain [17]. The aim of the present paper is to develop a theoretical model describing stress relaxation by the generation of rectangular prismatic dislocation loops (PDLs) at the interface in core-shell NWs with cores in the form of a long parallelepiped.

2. Model
Let us consider a composite NW as an elastic core-shell cylinder of radius $R$ with a core in the form of a long parallelepiped with a square cross section $(2a \times 2a)$. The mismatch of core and shell lattices is characterized by the misfit parameter $f = 2(a_c - a_s) / (a_c - a_s)$, where $a_c$ and $a_s$ are the lattice parameters...
of the core and shell materials, respectively. We assume that the core and shell materials have the same elastic modules. We also suppose that rectangular PDLs with sizes $2c \times 2h$ can appear in different regions of the core-shell interface (figure 1), in which cases they are denoted as follows: PDL-1 is generated from the middle of the interface and expands to the bulk of the core, PDL-2 is generated from the edge of the interface and also expands to the bulk of the core, and PDL-3 is generated from the middle of the interface and expands to the free surface of the NW.

$\begin{align*}
\Delta W &= W_2 - W_1 = W_c + W_{cl} + W_{int} < 0, \\
W_c &= 4(h + c) \frac{Db^2}{2},
\end{align*}$

$\begin{align*}
W_{cl} &= Db^2 \left( 2c \ln \frac{4c}{r_0} + 2h \ln \frac{4h}{r_0} - c \ln \frac{K + c}{K - c} - h \ln \frac{K + h}{K - h} - 4(c + h - K) \right),
\end{align*}$

where $D = G/(2\pi(1-\nu))$, $G$ is the shear modulus, $\nu$ is the Poisson ratio, $b$ is the Burgers vector magnitude for the PDL, $r_0$ is the core radius of the PDL, and $K = \sqrt{c^2 + h^2}$.

The core energy of a rectangular PDL is approximated by [19] as:

$W_{int} = -b \int_{a}^{a+2c} dx \int_{h}^{h} \sigma_{zz} dy$,

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The misfit stress $\sigma_{zz}$ was found in a closed analytical form in [17]. In the case shown in figure 1, it can be written as follows:

$\sigma_{zz} = C \pi \text{ sign} \left( \frac{x-x_0}{y-y_0} \right) + 8\frac{R^2}{r^2} \left( 2xy \ln \sqrt{R^4 - 2R^2(xx_0 + yy_0) + (x^2 + y^2)(x_0^2 + y_0^2)} + \right.$

Figure 1. Generation of rectangular PDLs in a cross section of a core-shell NW with a parallelepiped core. We consider three possible cases for the PDL generation at the interface: (1) from the middle of the flat interface into the core, PDL-1; (2) from the core edge into the core, PDL-2; and (3) from the middle of the flat interface to the free surface, PDL-3.
\( + (x^2 + y^2) \arctg \left( \frac{x_0y - xy_0}{R^2 - x_0y - xy_0} \right) \left| \begin{array}{l} x_0 = a \\ y_0 = 0 \\ x = a \\ y = 0 \end{array} \right. \),

(5)

where \( C = f G (1 + \nu) / [2\pi (1 - \nu)] \). Using Eq. (5), the interaction energies (4) were calculated numerically. Thus, we determined all the terms appearing in equation (1).

3. Results

To study the energy change of an NW due to the generation of rectangular PDLs at the interface, we used the energy maps built in the phase space of the normalized PDL sizes of \( 2a/b \) and \( 2c/b \). Following [13], we considered two cases of Si/Ge \((f = 0.042)\) and InAs/ZnS \((f = 0.107)\) core-shell NWs for \( R = 100 \text{ nm} \) and \( a = 0.5R = 50 \text{ nm} \) (figure 2). As figure 2(a) demonstrates, the generation of PDL-1 and PDL-2 in Si/Ge core-shell NWs is energetically unfavorable. In contrast, the generation of these PDLs in the InAs/ZnS core-shell NWs (figure 2(b)) is energetically favorable even for very

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**Figure 2.** Maps of the energy change \( \Delta W \) in the space of normalized sizes of PDLs \( 2a/b \) and \( 2c/b \) for Si/Ge (a,c) and InAs/ZnS (b,d) core-shell NWs for \( R = 100 \text{ nm} \) and \( a = 0.5R = 50 \text{ nm} \). (a,b) is the case of either PDL-1 or PDL-2; (c,d) is the case of PDL-3. The energy values are given in units of \( Gb^3 \).
small PDL sizes. The generation of PDL-3 is energetically unfavorable for both the Si/Ge (figure 2(c)) and InAs/ZnS (figure 2(d)) core-shell NWs.

The misfit parameter $f$ is in direct proportion to the interaction energy (5). Therefore, it is easily extracted from the equation $\Delta W = 0$, which determines the critical conditions needed for the generation of PDLs. This generation becomes energetically favorable ($\Delta W < 0$) if $f$ exceeds a critical value $f_c$, which depends on the core and shell sizes, as well as on the type and sizes of the PDL. Figure 3 shows these dependences for different types of PDLs, which are calculated from the equation:

$$f_c = \frac{W_c + W_r}{W_{\text{int}}},$$

(6)

where $W_{\text{int}}^* = -W_{\text{int}} / f$.

It is seen from figure 3 that generation of PDL-2 requires the smaller values of the critical misfit $f_c$, which means that this type of PDL is preferable over the other two. It is also seen that $f_c$ increases with $a$ for PDL-1 and PDL-2 at a fixed value of $R$. Indeed, an increase in the core size leads to a decrease in the axial misfit stress in the core and, therefore, in the term $W_{\text{int}}^*$ appearing in the balance (6). As a result, the critical misfit $f_c$ must increase. In contrast, $f_c$ decreases with $a$ for PDL-3 at a fixed value of $R$. This is so because increasing the core leads to increasing the axial misfit stress in the shell and, therefore, to increasing the term $W_{\text{int}}^*$. It is also worth noting that $f_c$ decreases with an increase in $R$ at a constant $a$ for PDL-1 and PDL-2, and, conversely, for PDL-3, due to similar reasons.

![Figure 3](image_url)

**Figure 3.** Dependence of the critical misfit $f_c$ on the core size $a$ for different values of radius $R$ (in nanometers) at $c/h = 0.2$, $h/b = 10$, and $b = 0.3$ nm. Black, magenta and red curves correspond to PDLs of types 1, 2 and 3, respectively.

4. Conclusions
A theoretical model is suggested which describes misfit stress relaxation in core-shell NWs with symmetric parallelepiped cores by the generation of rectangular PDLs at the core-shell interface. Three different types of PDLs are considered which are generated either in the middle or on the edge of the flat interface and expand either to the bulk of the core or to the free surface of the NW. It is shown that PDLs generated on the core edge and expanding into the bulk of the core are the most preferable PDLs for the NWs. For these PDLs, the critical misfit $f_c$ increases with the core size $a$ and decreases with the NW radius $R$. 
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