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The Role of Interface Sharpness in the Formation of Misfit Dislocations in Core-Shell Nanowires

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Abstract

An analytical model for the nucleation of edge misfit dislocations in cylindrical core-shell nanowires with a diffuse interface boundary is developed. The model is formulated within the framework of linear isotropic elasticity theory and accounts for the interplay between the nanowire's geometry, interface diffuseness, and lattice mismatch. By evaluating the total energy change associated with dislocation formation, we systematically analyze the dependence of energetic favorability of dislocation nucleation on the core/shell radius ratio, diffuse interface width, and misfit parameter. The results demonstrate that sharp interfaces maximize the energy gain from dislocation formation, whereas diffuse interfaces suppress it, particularly in nanowires with thin cores. The optimal dislocation nucleation site is primarily governed by geometry features and only weakly influenced by misfit parameter. A critical misfit parameter is identified, above which the nanowire coherent state becomes unstable. The analysis reveals that while broader diffuse interfaces reduce the tendency for relaxation process, increased lattice mismatch promotes it.

Keywords: Core-shell nanowire; Diffuse interface; Misfit dislocations; Misfit stress relaxation

1. INTRODUCTION

Light-emitting devices based on one-dimensional heterostructures offer several key advantages over conventional planar heterostructures, including crystal defect density, enhanced light extraction efficiency, increased effective light-emitting surface area, and superior control over charge carrier density and injection [1,2]. A typical example of such one-dimensional heterostructures is core-shell nanowires (NWs). A range of synthesis methods can be employed to fabricate such heterostructures, such as the vapor-liquid-solid method, metalorganic chemical vapor deposition method, electrochemical deposition method, colloidal chemistry approaches, etc. [3–5]. The growth of core-shell NWs via almost all techniques is fundamentally a kinetically controlled process, far removed from thermodynamic equilibrium. Driving forces like high vapor supersaturation, rapid precursor switching, or an applied electric potential create conditions where the deposition rate of new atoms significantly exceeds their rate of relaxation into the most stable lattice sites. This imbalance between the material supply rate and its ordering rate leads to several interrelated phenomena that cause interface broadening. Consequently, the resulting interface is rarely atomically sharp. Instead, a diffuse interphase boundaries form, with a thickness ranging from a few to tens of nanometers, where the composition smoothly varies from the core material to the shell one [6,7].

While such a diffuse interface can sometimes be beneficial for reducing mechanical stress, it is often an undesirable compromise that degrades the heterostructure's electronic and optical properties, for instance, by smoothing out potential barriers in quantum wells or promoting carrier leakage [8,9]. Since the diffuse interface in NWs prevents the formation of misfit defects due to the reduction of the misfit strain energy [8,10], such effect should be considered in strict theoretical models describing misfit stress relaxation in core-shell NWs.

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To date, a significant number of theoretical studies have been devoted to describing the formation of circular and rectangular dislocation loops [11–20], straight dislocations [21,22], and their dipoles [23,24] in core-shell NWs with an atomically sharp interface. Research on the relaxation of mechanical stresses in heterostructures with diffuse interfaces has largely focused on axially-inhomogeneous nanowires [25–27]. A key reason for the paucity of theoretical models on stress relaxation in radially-inhomogeneous NWs with radial composition gradients has been the unavailability of a closed-form analytical solution for the elastic fields in such core-shell NWs. The recent advent of this solution [28] has enabled progress in this area.

Thus, the objective of this study is to develop an analytical model describing the nucleation of an edge misfit dislocation in a cylindrical core-shell NW featuring a diffuse interface. This model will be used to systematically investigate how the energetic preference for this nucleation process is affected by the heterostructure's geometry, the specific profile of the interface, and the material properties of the NW.

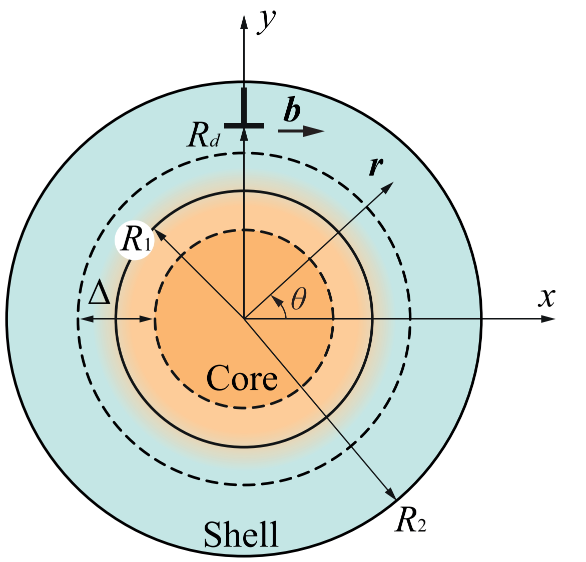

Fig. 1. A composite core-shell NW featuring an MD in the shell and a diffuse core-shell interface. R_1 is the radius of the NW core, R_2 is the outer radius of the NW, Δ is the thickness of the diffuse interface between the core and the shell, and R_d denotes the radial position of the MD within the NW.

2. MODEL

Consider a cylindrical core-shell NW with a radially diffuse heterointerface and a misfit dislocation (MD) whose line is parallel to the NW axis and shifted from it (see Fig. 1). Within the classical theory of linear elasticity for elastically isotropic and homogeneous medium, the total energy of the core-shell NW can be written as follows:

$$W = W_{st} + W_d + W_c + W_{int}, \tag{1}$$

where W_{st} is the strain energy of the NW with no MD, W_d is the strain energy of the MD, W_c is its core energy, and W_{int} is the energy of interaction between the MD and the misfit stress field in the NW.

Nucleation of a MD is considered energetically favorable if the total energy change of the NW associated with MD formation becomes negative [22]:

$$\Delta W = W - W_{st} = W_d + W_c + W_{int} < 0. \tag{2}$$

The MD core energy W_c can be estimated in the standard manner [29]:

$$W_c = \frac{Gb^2}{4\pi(1-\nu)}, \tag{3}$$

where G is the shear modulus, ν is the Poisson ratio, and b is the Burgers vector magnitude of the MD.

The MD strain energy W_d in a composite NW was derived analytically by integrating the relevant component of the stress field generated by displaced dislocation in an infinite cylinder using the Airy stress function approach [22]:

$$W_d = \frac{Gb^2}{8\pi(1-\nu)} \times \left\{ \frac{(t_d^2-1)(3+2r_0^3 t_d - 5t_d^2 + 2t_d^4 + r_0^2(6t_d^2-3) + r_0(6t_d^3 - 8t_d))}{(t_d^2 + r_0 t_d - 1)^2} + \ln\left[\frac{(t_d^2 + r_0 t_d - 1)^2}{r_0^2}\right] \right\}, \tag{4}$$

where $t_d = R_d / R_2$ is the normalized radial position of the MD in the NW, $r_0 = r_c / R_2$ is the normalized dislocation core radius, and R_2 is the outer radius of the NW.

The interaction energy W_{int} can be evaluated as the mechanical work required to introduce the MD in the misfit stress field of the NW:

$$W_{int} = -\int_{R_d}^{R_2} \sigma_{\theta\theta} dr. \tag{5}$$

For a NW with a diffuse core-shell interface, approximated by a piecewise-linear profile, the relevant stress component $\sigma_{\theta\theta}$ takes the form [28]:

$$\sigma_{\theta\theta}^{(1)} = \sigma_0 \left[-1 + t_0^2 + \frac{\delta^2}{12} \right], \quad 0 < t \le t_0 - \delta/2,$$

$$\sigma_{\theta\theta}^{(2)} = \sigma_0 \left[\frac{32t^3 + 2t^2(-12t_0 - 6\delta + 12t_0^2\delta + \delta^3) - (2t_0 - \delta)^3}{24t^2\delta} \right],$$

$$t_0 - \delta/2 < t \le t_0 + \delta/2,$$

$$\sigma_{\theta\theta}^{(3)} = \sigma_0 \left[\frac{(t^2+1)(12t_0^2 + \delta^2)}{12t^2} \right], \quad t_0 + \delta/2 < t \le 1, \tag{6}$$

where $\sigma_0 = f_0 G(1+\nu)/(1-\nu)$, $\delta = \Delta / R_2$ is the diffuse interface width normalized by the outer NW radius, $t = r / R_2$, and $t_0 = R_1 / R_2$.

Note that the local eigenstrain f in such an NW is defined as:

$$f(t) = f_0 \begin{cases} 1, & 0 < t \le t_0 - \delta/2, \\ (t_0 - t)/\delta + 0.5, & t_0 - \delta/2 < t \le t_0 + \delta/2, \\ 0, & t_0 + \delta/2 < t \le 1, \end{cases} \quad (7)$$

where f_0 is the misfit parameter characterizing the lattice mismatch between the core and shell materials in the NW.

Accordingly, the interaction energy W_{int} takes three distinct forms depending on the MD position:

for the MD position inside the core

$$W_{int}^{(1)} = -b\left(\int_{t_d}^{t_0-\delta} R_2\sigma_{\theta\theta}^{(1)} dt + \int_{t_0-\delta}^{t_0+\delta} R_2\sigma_{\theta\theta}^{(2)} dt + \int_{t_0+\delta}^{1} R_2\sigma_{\theta\theta}^{(3)} dt\right),$$

$$0 \le t_d < t_0 - \frac{\delta}{2}; \quad (8)$$

for the MD position inside the diffuse interface

$$W_{int}^{(2)} = -b\left(\int_{t_d}^{t_0+\delta} R_2\sigma_{\theta\theta}^{(2)} dt + \int_{t_0+\delta}^{1} R_2\sigma_{\theta\theta}^{(3)} dt\right),$$

$$t_0 - \frac{\delta}{2} \le t_d < t_0 + \frac{\delta}{2}; \quad (9)$$

and for the MD position inside the shell,

$$W_{int}^{(3)} = -b\int_{t_d}^{1} R_2\sigma_{\theta\theta}^{(3)} dt, \; t_0 + \frac{\delta}{2} \le t_d \le 1. \quad (10)$$

By evaluating the integrals (8)–(10), one obtains the final closed-form expression for the interaction energy W_{int}:

$$W_{int} = -\sigma_0 b R_2 \begin{cases} \dfrac{t_1 - t_a}{24\delta}\left(16(t_1 + t_a) + 2C - \dfrac{D}{t_1 t_a}\right) - \dfrac{A(t_1^2 - 1)}{12 t_1} + B(t_a - t_d), & 0 \le t_d \le t_a, \\ \dfrac{t_1 - t_d}{24\delta}\left(16(t_1 + t_d) + 2C - \dfrac{D}{t_1 t_d}\right) - \dfrac{A(t_1^2 - 1)}{12 t_1}, & t_a < t_d < t_1, \\ -\dfrac{A(t_d^2 - 1)}{12 t_d}, & t_1 \le t_d \le 1, \end{cases} \quad (11)$$

where $A = 12t_0^2 + \delta^2$, $B = -1 + t_0^2 + \delta^2/12$, $C = -12t_0 - 6\delta + 12t_0^2 + \delta^3$, $D = (2t_0 - \delta)^3$, $t_1 = (t_0 + \delta/2)$, $t_a = (t_0 - \delta/2)$.

Thus, all terms of Eq. (2) have been determined.

3. RESULTS AND DISCUSSION

The calculations utilized a core-shell NW model featuring a piecewise-linear radial eigenstrain profile with these parameters: modulus of Burgers vector $b = 0.4$ nm, shell radius $R_2 = 100b$, Poisson's ratio $\nu = 0.31$, and shear modulus $G = 48$ GPa. The misfit parameter f_0 and the core radius R_1 were varied during the work, with their specific values indicated in the descriptions of each considered configuration. The distribution of total energy change ΔW depends on the misfit parameter f_0, the normalized interface width δ, the normalized radial coordinate of edge dislocation nucleation t_d, and core-shell radius ratio R_1 / R_2.

For a NW with a thin core and a thick shell ($R_1 / R_2 = 0.3$, Fig. 2a), the relatively sharp interface with $\delta = 0.1$ (blue curve) leads to the most pronounced reduction in the total energy change ΔW due to the MD nucleation. The energy minimum is $\Delta W_{min} \approx -0.34Gb^2$ at the MD position $t_d \approx 0.26$. For an intermediate interface width $\delta = 0.3$ (orange curve) the magnitude of the energy change reduction becomes noticeably smaller, with the minimum $\Delta W_{min} \approx -0.16Gb^2$ at $t_d = 0.28$. The energy change profile becomes more gradual, without abrupt kinks. For the most diffuse interface with $\delta = 0.5$ (green curve), the energy change becomes notably shallower and broader, attaining the minimum value $\Delta W_{min} \approx -0.06Gb^2$ at $t_d = 0.34$. In the case of a perfectly sharp interface ($\delta = 0$, red curve), the energy change minimum is the deepest, $\Delta W_{min} \approx -0.48Gb^2$ at $t_d = 0.3$, as one could expect in advance. It is worth noting that only for the perfectly sharp interface with $\delta = 0$, the energy change minimum ΔW_{min} lies strictly at the boundary of the pure core region. For a slightly diffuse interface with $\delta = 0.1$, the minimum is shifted inward the pure core region, while for broader diffuse interfaces with $\delta = 0.3$ and 0.5, the minimum is located within the diffuse interface itself and progressively shifts toward the shell with an increase in δ.

In the case of a NW with equal core radius and shell thickness ($R_1 / R_2 = 0.5$, Fig. 2b), a relatively sharp interface with $\delta = 0.1$ (blue curve) leads to the total energy change minimum $\Delta W_{min} \approx -1.01Gb^2$ at $t_d \approx 0.45$. For a less sharp interface with $\delta = 0.3$ (orange curve), the minimum becomes smoother, with $\Delta W_{min} \approx -0.68Gb^2$ at $t_d \approx 0.38$, while a further increase in the interface blurriness up to $\delta = 0.5$ (green curve) leads to an even smoother and shallower minimum with $\Delta W_{min} \approx -0.42Gb^2$ at $t_d \approx 0.39$. In the case of a perfectly sharp interface with $\delta = 0$ (red curve), the minimum is $\Delta W_{min} \approx -1.18Gb^2$ at $t_d = 0.5$. As

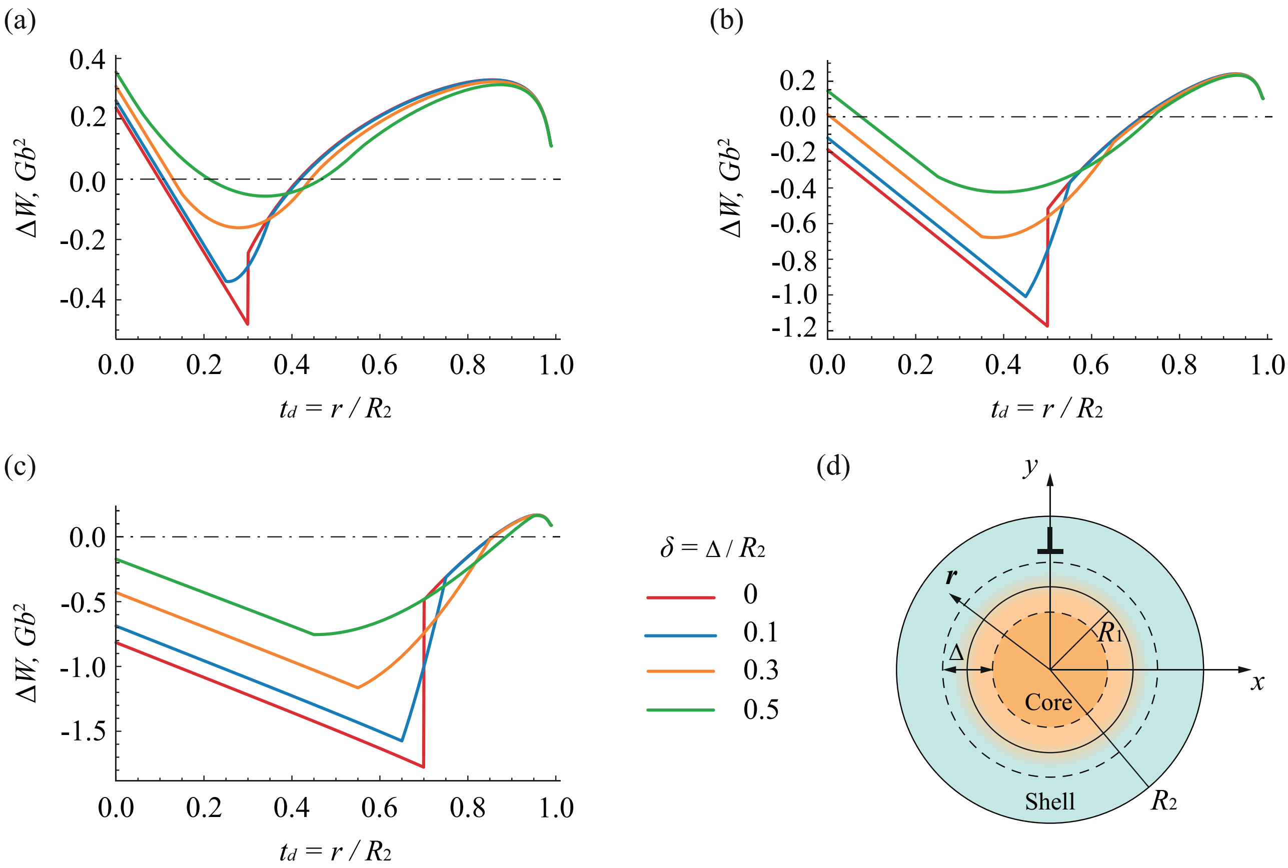

Fig. 2. Dependences of the total energy change ΔW on the normalized radial coordinate t_d of an MD in core-shell NWs with various values of the position and width of the diffuse interface for $f_0 = 0.05$ and $R_1 / R_2 = 0.3$ (a), 0.5 (b), and 0.7 (c). The red, blue, orange, and green curves correspond to the normalized interface widths $\delta = 0$, 0.1, 0.3, and 0.5, respectively. Panel (d) presents a sketch of the dislocated NW cross section. The values of ΔW are given in units of Gb^2.

follows from these observations, at $R_1 / R_2 = 0.5$, the minimum position is strictly at the core boundary when the interface is perfectly sharp with $\delta = 0$. For a diffuse interface, the minimum is shifted inward the pure core region if $\delta = 0.1$ (as is also the case with $R_1 / R_2 = 0.3$, Fig. 2a), while it resides within the diffuse interface at practically the same positions for $\delta = 0.3$ and 0.5.

In the case of a NW with a thick core and a thin shell ($R_1 / R_2 = 0.7$, Fig. 2c), the situation is a bit different. For a relatively sharp interface with $\delta = 0.1$ (blue curve), the total energy change has the minimum $\Delta W_{min} \approx -1.58Gb^2$ at $t_d \approx 0.65$. For a more diffuse interface with $\delta = 0.3$ (orange curve), $\Delta W_{min} \approx -1.16Gb^2$ at $t_d \approx 0.55$, and for the most diffuse interface with $\delta = 0.5$ (green curve), the minimum shifts inward and becomes $\Delta W_{min} \approx -0.75Gb^2$ at $t_d \approx 0.45$. In the case of a perfectly sharp interface with $\delta = 0$ (red curve), the minimum is $\Delta W_{min} \approx -1.78Gb^2$ at $t_d = 0.7$. Again, in the case of a diffuse interface, the minimum is shifted inward the pure core region if $\delta = 0.1$ (as was before with $R_1 / R_2 = 0.3$ and 0.5, Figs. 2a,b), it is located within the diffuse interface, however progressively shifts toward the core with an increase in δ, in contrast with the previous cases of $R_1 / R_2 = 0.3$ and 0.5.

Bringing together the trends observed in Figs. 2a–c, Figure 3 shows how the optimal position $t_{d,opt}$ of the MD, which corresponds to the total energy change minimum

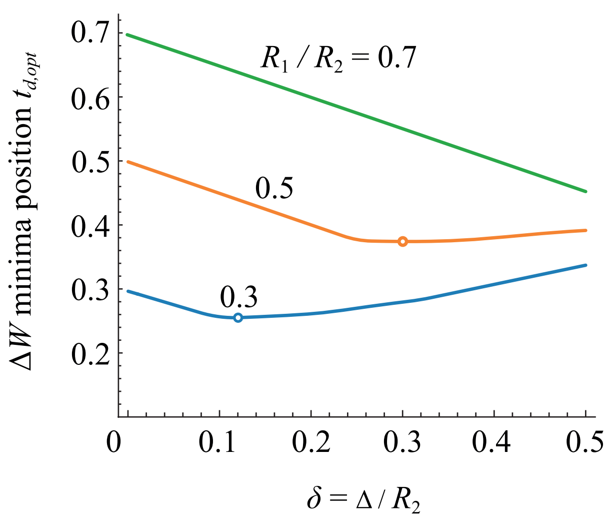

Fig. 3. Dependences of the normalized optimal position $t_{d,opt}$ of the MD on the normalized interface width δ for $f_0 = 0.05$ and different values of the R_1 / R_2 ratio. Circles mark the minima of the blue and orange curves.

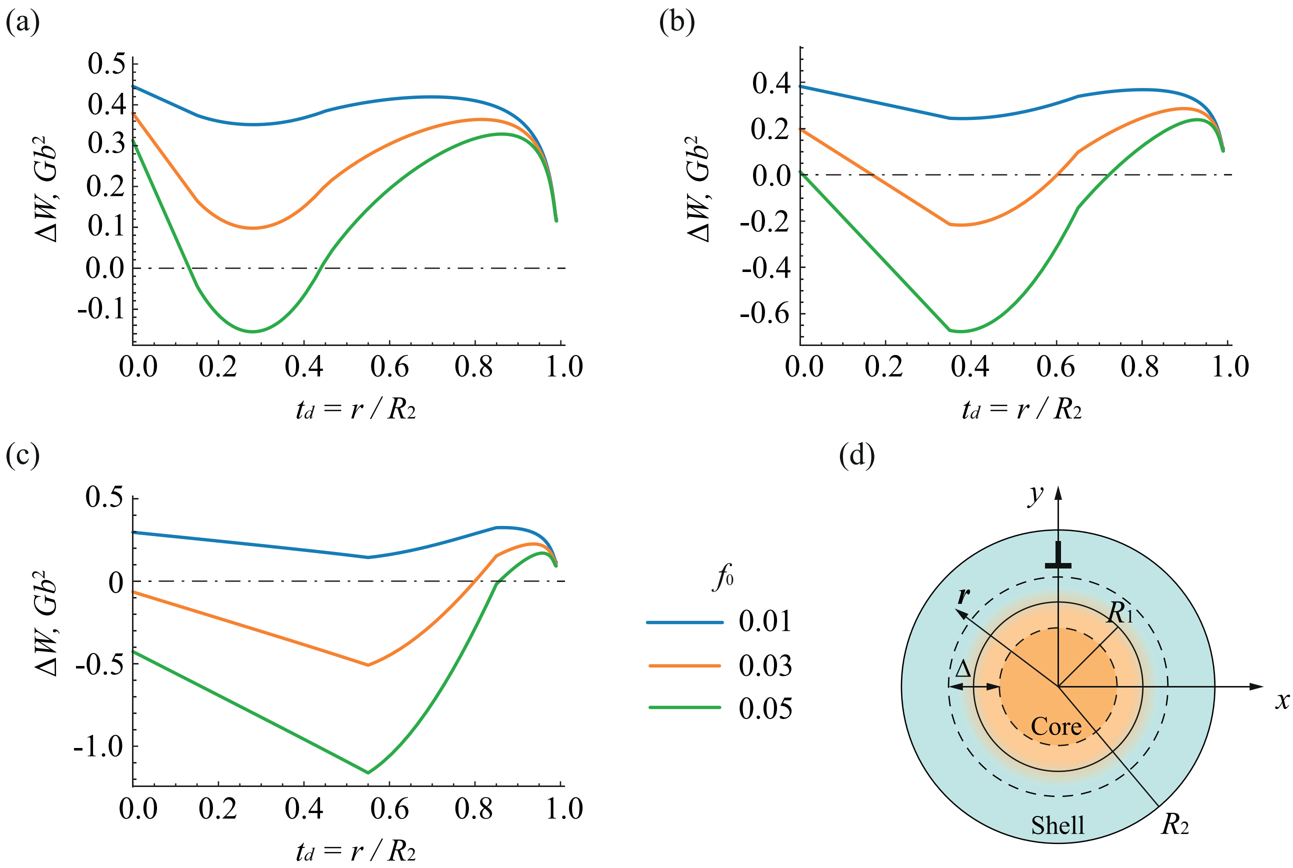

Fig. 4. Dependences of the total energy change ΔW on the normalized radial coordinate t_d of an MD in core-shell NWs for $\delta = 0.3$ and $R_1 / R_2 = 0.3$ (a), 0.5 (b), and 0.7 (c). The blue, orange, and green curves correspond to the misfit parameter values $f_0 = 0.01$, 0.03, and 0.05, respectively. Panel (d) presents a sketch of the NW cross section. The values of ΔW are given in units of Gb^2.

ΔW_{min}, responds to changes in the interface width δ for the considered NW geometries at fixed $f_0 = 0.05$.

For a NW with a thin core and a thick shell ($R_1 / R_2 = 0.3$, Fig. 3, blue curve), the optimal MD position $t_{d,opt}$ is located precisely at the core-shell boundary ($t_{d,opt} = 0.3$) when $\delta = 0$. As δ increases to ~ 0.11, this position shifts maximally inward the core, with $t_{d,opt} \approx 0.25$. Beyond this point ($\delta > 0.11$), the trend reverses and $t_{d,opt}$ gradually moves outward, with its limiting value ~ 0.34 at $\delta = 0.5$. As with the blue curve, the orange curve ($R_1 / R_2 = 0.5$) shows a comparable pattern. In this case, $t_{d,opt}$ reaches its minimum ~ 0.38 at $\delta = 0.3$ and its limiting value ~ 0.39 at $\delta = 0.5$. In contrast, the green curve ($R_1 / R_2 = 0.7$) linearly decreases with varying $t_{d,opt}$ from 0.7 at $\delta = 0$ to ~ 0.45 at $\delta = 0.5$. Interestingly, all the three curves are linear in some range of δ, at its small values for $R_1 / R_2 = 0.3$ and 0.5, and in all the range of δ for $R_1 / R_2 = 0.7$. Moreover, the slopes of these linear parts of the curves are almost equal.

The influence of the misfit parameter f_0 on the total energy change ΔW of the dislocated NW with the normalized interface width $\delta = 0.3$ and the radii ratios $R_1 / R_2 = 0.3$, 0.5, and 0.7 is illustrated by Fig. 4.

As is seen from Fig. 4, the smallest misfit value $f_0 = 0.01$ is not enough for MD formation since $\Delta W > 0$ for any value of the R_1 / R_2 ratio under consideration. For a higher misfit value (here for $f_0 = 0.03$), no MD can form at $R_1 / R_2 = 0.3$, however its formation is possible at $R_1 / R_2 = 0.5$ and 0.7. The highest misfit value $f_0 = 0.05$ obviously provides the MD formation for any value of the R_1 / R_2 ratio.

For a NW with a thin core and a thick shell ($R_1 / R_2 = 0.3$, Fig. 4a), the highest misfit $f_0 = 0.05$ gives $\Delta W_{min} \approx -0.16Gb^2$ at $t_d \approx 0.28$. When the NW has equal core radius and shell thickness ($R_1 / R_2 = 0.5$, Fig. 4b), the energy change minimum ΔW_{min} is at $t_d \approx 0.38$ and roughly equal to $-0.22Gb^2$ at $f_0 = 0.03$ and $-0.68Gb^2$ at $f_0 = 0.05$. For a NW with a thick core and a thin shell ($R_1 / R_2 = 0.7$, Fig. 4c), ΔW_{min} is at $t_d \approx 0.55$ and roughly equal to $-0.51Gb^2$ at $f_0 = 0.03$ and $-1.164Gb^2$ at $f_0 = 0.05$. Thus, with $\delta = 0.3$, the optimal MD position $t_{d,opt}$ is always within the diffuse interface region for any value of the R_1 / R_2 ratio, however it gradually shifts to the periphery of the NW with an increase in R_1. Interestingly, the normalized equilibrium distance $d_{eq} = R_1 / R_2 - t_{d,opt}$ increases as well, from ~ 0.02 at $R_1 / R_2 = 0.3$ to ~ 0.12 at $R_1 / R_2 = 0.5$, and ~ 0.15 at $R_1 / R_2 = 0.7$.

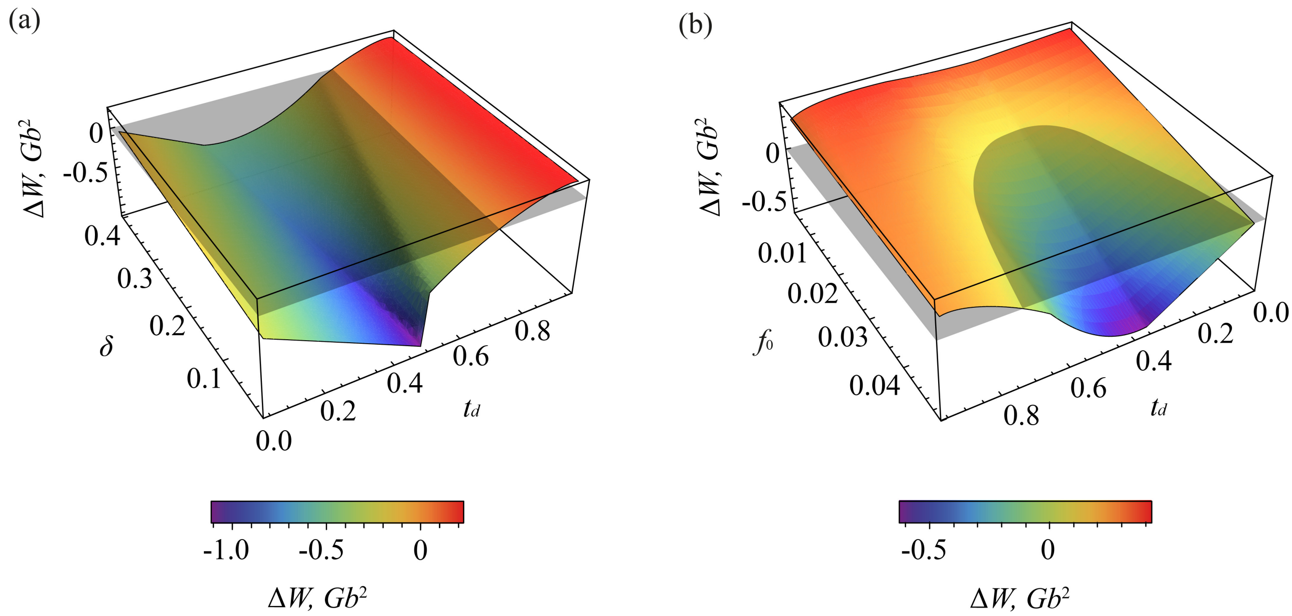

Fig. 5. The 3D maps of the total energy change ΔW in the space of (a) the normalized radial position t_d of an MD and the normalized interface width δ at $f_0 = 0.05$, and (b) t_d and the misfit parameter f_0 at δ = 0.3. The core and shell radii ratio is $R_1 / R_2 = 0.5$. The grey plane shows the zero value of ΔW. The values of ΔW are given in units of Gb^2.

Figure 5 presents 3D maps of the total energy change ΔW in the (t_d, δ) and (t_d, f_0) parameter spaces for the case of $R_1 / R_2 = 0.5$.

As is seen from Fig. 5a, as δ increases, the ΔW minimum located in the diffuse interface region becomes shallower and smoother. When the MD is within the shell region, ΔW remains higher than at any MD position inside the core or the diffuse interface; thus, the formation of an MD in the NW shell is energetically unfavorable. A clear shift of the ΔW minimum toward the NW center is observed with increasing δ, which is consistent with the energy change behavior shown in Fig. 2b.

Analysis of Fig. 5b shows that, at small values of the misfit parameter f_0, the MD formation is energetically unfavorable in any part of the NW. As the misfit increases, the energy change minimum ΔW_{min} appears in the diffuse interface region, in agreement with the energy change behavior shown in Fig. 4b. As is the case with Fig. 4a, ΔW in Fig. 5b takes the highest values throughout the shell region for all f_0 values under consideration, thus confirming the earlier conclusion that the MD formation in the NW shell is the least energetically favorable scenario for misfit stress relaxation.

The 2D maps of the critical misfit parameter f_c, at which the total energy change ΔW associated with the MD nucleation becomes zero ($\Delta W = 0$), are presented in Fig. 6 in the spaces (t_d, δ) at the normalized shell thickness $h = 1 - R_1 / R_2 = 0.5$ (Fig. 6a) and (t_d, h) at δ = 0.3 (Fig. 6b). The critical misfit value f_c separates two distinct states of the NW: for $f_0 < f$, the core/shell interface remains coherent (with no MDs), whereas for $f_0 > f_c$, the MD formation becomes energetically favorable.

As is seen from Fig. 6a, the minimum value of f_c, $f_{c,min} \approx 0.016$, corresponds to the MD position $t_d \approx 0.45$, thus confirming the earlier observation that the optimal MD position does not coincide with the center of the diffuse interface ($R_1 / R_2 = 0.5$) but is shifted from it by the normalized equilibrium distance $d_{eq} \approx 0.05$ toward the pure core region. When the MD is shifted toward the NW free surface, f_c gradually increases, while its shift toward the NW core results in a significantly slower rise in f_c. This trend further supports the conclusion that the shell region is less energetically favorable for the MD nucleation.

Figure 6b shows that lower f_c values are characteristic of NWs with thin shells. As h increases, the f_c contours shift upward and become more closely spaced, indicating that the MD nucleation becomes progressively less favorable. The widest ranges of the MD position t_d corresponding to low f_c values are observed in NWs with larger cores. The t_d value associated with the minimum f_c is displaced toward the center of the NW core with increasing h.

4. CONCLUSIONS

In this work, an analytical model is proposed that describes the nucleation of a MD in a core-shell NW with a diffuse interface. The model is developed within the framework of an energy-based approach using the approximation of the linear homogeneous elasticity theory. It is shown that the energetic favorability of MD formation in the core-shell NW is strongly governed by the system geometry, characterized by the core and shell radii ratio R_1 / R_2. For very thin cores covered with thick shells, the NW remains

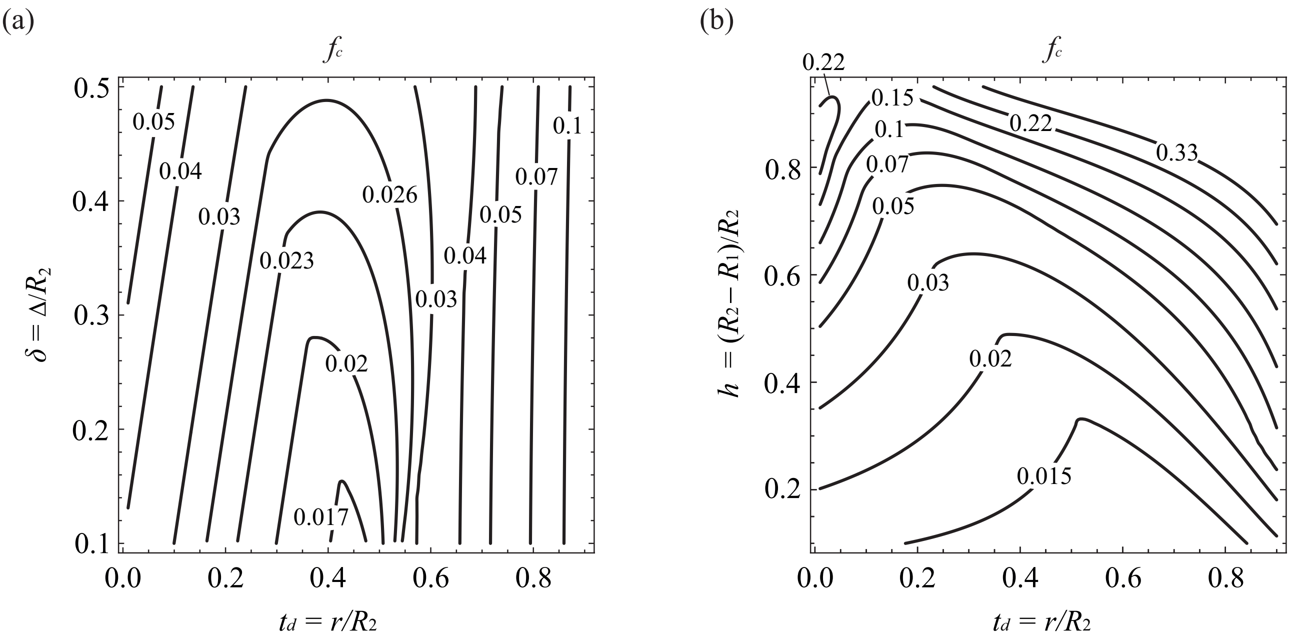

Fig. 6. The maps of the critical misfit parameter f_c in the space of (a) the normalized radial position t_d of the MD and the normalized interface width δ at $h = 0.5$, and (b) t_d and the normalized shell thickness h at $\delta = 0.3$.

predominantly in the coherent state with no MDs, whereas for larger cores, the misfit relaxation via the MD nucleation becomes energetically preferred, as is also the case with a perfectly sharp core/shell interface.

Relatively sharp diffuse interfaces (here with $\delta = 0.1$) maximize the energy gain associated with MD formation, while broader diffuse interfaces (here with $\delta = 0.5$) significantly suppress this effect. This trend is particularly pronounced for NWs with small cores. The optimal MD position weakly depends on the misfit parameter f_0, indicating that it is primarily determined by the radii ratio R_1 / R_2, and secondarily by the normalized interface width δ.

A critical misfit value f_c is identified, above which the coherent state of NW becomes unstable with respect to MD nucleation. This critical value decreases as the core becomes larger. Furthermore, the radial range favorable for the MD nucleation broadens with an increase in the misfit parameter f_0, implying that, under a sufficiently high misfit, MDs may nucleate not only within the core but also within the shell.

In conclusion, our analysis has revealed a competitive interplay between the interface width δ and the misfit parameter f_0: while a broader interface suppresses the energetic favorability for MD formation, an increased lattice mismatch promotes it.

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Роль резкости границы раздела в формировании дислокаций несоответствия в нанопроволоках типа «ядро-оболочка»

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Аннотация. Разработана аналитическая модель зарождения краевых дислокаций несоответствия в цилиндрических нанопроволоках типа «ядро-оболочка» с размытой границей раздела. Модель построена в рамках линейной изотропной теории упругости и учитывает взаимосвязь между геометрией нанопроволоки, степенью размытости границы раздела и параметром несоответствия решёток материалов нанопроволоки. Проведён систематический анализ зависимости энергетической предпочтительности образования дислокации несоответствия от отношения радиусов ядра и оболочки, ширины диффузной границы и параметра несоответствия. Показано, что резкие границы максимизируют выигрыш в энергии при образовании дислокации, тогда как диффузные границы подавляют этот процесс, особенно в нанопроволоках с малым ядром. Оптимальное положение зарождения дислокации в первую очередь определяется геометрическими особенностями нанопроволоки и слабо зависит от параметра несоответствия. Определён критический параметр несоответствия, превышение которого может приводить к нарушению когерентного состояния нанопроволоки. Установлено, что широкая размытая граница в нанопроволоке снижает вероятность образования дислокаций несоответствия, а увеличение параметра несоответствия между кристаллическими решётками ядра и оболочки способствует этому процессу.

Ключевые слова: нанопроволока типа «ядро-оболочка»; размытая граница раздела; дислокации несоответствия; релаксация напряжений несоответствия