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Self-energy of elliptical dislocation loops in anisotropic crystals and its application for defect-free core/shell nanowires

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Abstract

In this work we investigate the self-energy of elliptical dislocation loops in anisotropic crystals and determine the functional dependencies on loop circumference, shape, and dislocation core radius. Systematic numerical calculations using the anisotropic point force Green's function method are carried out with the goal of developing an analytical expression for the self-energy associated with these loops. The resulting formula is shown to accurately predict the self-energies for elliptical loops in anisotropic crystals, as well as the self-energies for simple loop configurations in isotropic crystals, for which analytical expressions exist. We apply this expression to predict the critical shell thickness corresponding to defect-free core/shell nanowires (NW) and further for the first time consider the effect of image energy due to the finite size of NW in anisotropic media using the boundary element method. Consequently, self-energy in NWs is corrected by an energy factor. Moreover, we discuss the dependence of the critical shell thickness on growth direction, with ⟨1 1 0⟩ NW having the largest, ⟨1 1 1⟩ NW the next largest, and ⟨1 1 2⟩ NW the finest.
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1. Introduction

The lattice mismatch and thermal mismatch between adjacent materials often result in internal strains during the syntheses of nanostructures, such as core/shell nanowires (NW) [1–8] and coating/multilayer nanostructures [9–12], that could be partially/fully relaxed via the formation of misfit/threading dislocations [1–12]. Such misfit dislocation loops have been observed by high resolution transmission electron microscopy (HRTEM), for instance, at the interface of GaN/GaP NW [2]. These defects can negatively affect the physical behavior [12–18], e.g. mechanical strength [15–17], features of the electric and optical spectra [12,18], and nanostructure synthesis, e.g. crystal growth [19,20] and formation of kinked NW [21–23]. In particular, as misfit dislocation density increases the electrical and optical properties of semiconductor nanostructures often deteriorate. This is a problem of considerable importance in the fabrication and design of core/shell semiconductor NW [24], which have generated much interest due to their high electron mobility and potential for use in future nanoelectronic and nanophotonic devices [25], e.g. nanowire field effect transistors [26].

It is well known that defect formation in core/shell NW is an instability triggered by the difference in lattice constants between materials used for the core and shell [27,28]. When the shell is first deposited the interface between the shell and core is coherent and free of defects. Coherency is accomplished by elastic straining of the lattices joined at the interface. The strains develop in the core and shell regions, and as the (defect-free) shell thickens the associated strain energies grow. If a misfit dislocation loop were introduced into the shell, as shown in Fig. 1, it could

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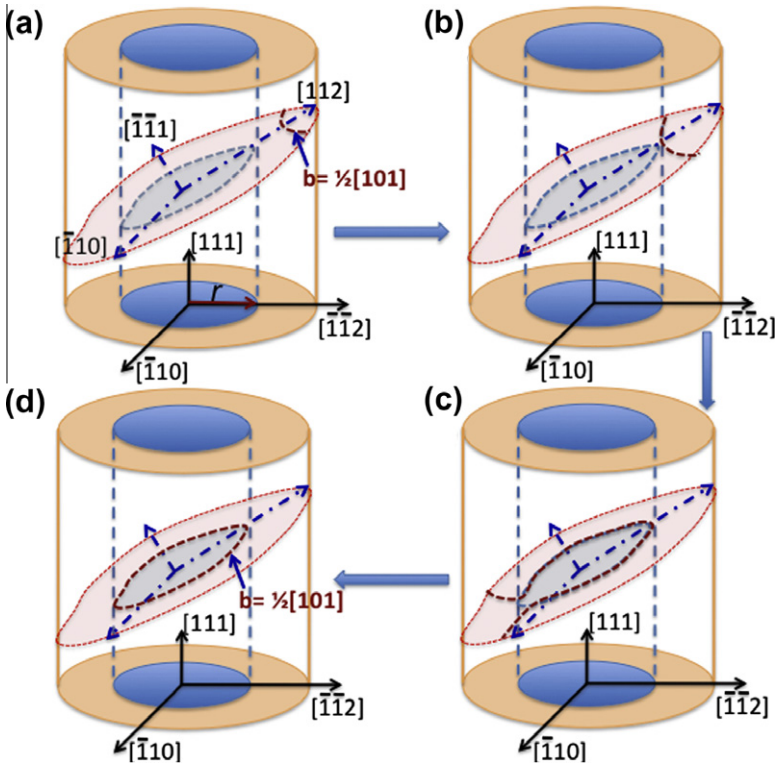

Fig. 1. Mechanism for misfit dislocation formation to relax the lattice mismatch strain in core/shell nanowires. The red dashed line represents the $\frac{1}{2}[1\,0\,1](\bar{1}\,\bar{1}\,1)$ dislocation loop. (a) Nucleation on the side surface of the shell, (b) propagation to the core/shell interface, (c) blocking of part of the dislocation loop at the interface, and finally (d) misfit dislocation loop formation around the interface. The misfit dislocation loop takes on an elliptical shape where the ratio between the major radius and the minor radius is determined by the angle θ between the glide plane and the growth direction. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

accommodate the lattice mismatch and reduce the misfit strains there. This reduction in strain, however, comes at the energetic expense of forming the loop. A stable misfit dislocation loop will form when the shell reaches a critical thickness beyond which the elastic strain energy in the shell due to the misfit strains exceeds the formation energy of the loop. In other words, under these conditions the presence of misfit dislocation loops reduces the overall strain energy relative to the defect-free state.

Predicting the critical thickness of the shell requires knowledge of the formation energy of the misfit dislocation loop, which depends on the loop size, shape, and Burgers vector. As illustrated in Fig. 1, a loop nucleates from the surface (Fig. 1a) onto {1 1 1} plane, propagates to the interface (Fig. 1b and c), and is then incorporated at the core/shell interface (Fig. 1d) as a misfit dislocation loop. The misfit dislocation loop has an elliptical shape that depends on the angle θ between the NW long axis (the growth direction) and the dislocation glide plane. Its minor radius r_a is equal to the radius of the core r_c, and its major radius r_b which is equal to $r_c/\cos\theta$. For example, for Ge/Si core/shell NW with a $\langle 1\,1\,1\rangle$ growth direction and a dislocation loop lying on a {1 1 1} plane in Si θ is 70.5°. The strain energy in the concentric cylinder core/shell configuration due to the lattice mismatch can be estimated, however, to date the energy of a dislocation loop of arbitrary shape (r_b/r_a) and circumference, lying at the interface between two dissimilar anisotropic crystals, has not been evaluated. Due to the complexity of the problem, it suffices to consider the strain energy stored by the same loop in an infinite anisotropic medium, a situation that also does not have an analytical expression. Analytical expressions only exist for a very few special dislocation loop configurations in isotropic crystals [29,31].

By applying a recently developed point force Green's function method [32–34] we for the first time develop an analytical formula for the self-energy of an elliptical dislocation in an anisotropic crystal as a function of its shape, size, and dislocation core radius. Using this expression we calculate the critical shell thickness for defect-free core/shell nanowires as the first order estimation. Further, we adopt a boundary element method (BEM) to calculate the image energy for NW that arises from the free surface and the finite size. Correspondingly, an energy factor that corrects the self-energy of a dislocation loop in an infinite domain is introduced to take care of the size effect. The results indicate that the critical shell thickness depends on the growth direction, with $\langle 1\,1\,1\rangle$ NW providing the largest defect-free shell thickness.

2. Methodology

The problem of interest is to obtain an expression for the distortion energy, more commonly referred to as the