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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.

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