Thermodynamic driving force in the formation of hexagonal-diamond Si and Ge nanowires

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Abstract: The metastable hexagonal-diamond phase of Si and Ge (and of SiGe alloys) displays superior optical properties with respect to the cubic-diamond one. Based on first-principle calculations we show that the surface energy of the typical facets exposed in Si and Ge nanowires is lower in the hexagonal-diamond phase than in the cubic one. By exploiting a synergic approach based also on a recent state-of-the-art

interatomic potential and on a simple geometrical model, we investigate the relative stability of nanowires in the two phases up to few tens of nm in radius, highlighting the surface-related driving force and discussing its relevance in recent experiments. We also explore the stability of Si and Ge core-shell nanowires with hexagonal cores (made of GaP for Si nanowires, of GaAs for Ge nanowires). In this case, the stability of the hexagonal shell over the cubic one is also favored by the energy cost associated with the interface linking the two phases. Interestingly, our calculations indicate a critical radius of the hexagonal shell much lower than the one reported in recent experiments, indicating the presence of a large kinetic barrier allowing for the enlargement of the wire in a metastable phase.

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