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Lattice Dynamics of Epitaxial Strain-Free Interfaces

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We studied the phonon properties of ultrathin Fe3Si layers in Ge/Fe3Si/GaAs heterostructures as a model system for epitaxial, strain-free interfaces. Epitaxial Fe3Si layers with thicknesses from 3ML to 36ML were grown on GaAs(001) substrates and capped by a 4 nm thick amorphous Ge layer. Sample characterization with various methods showed the formation of epitaxial Fe3Si nanostructures with perfect stoichiometry and high interface quality. Nuclear Inelastic Scattering was used to determine the iron-partial phonon density of states at room temperature as a function of layer thickness. The results exhibit up to a two-fold enhancement of the low-energy phonon states compared to the bulk material for layer thicknesses of 8 monolayers and below. First-principles calculations explain the observed effect by novel, interface-specifc phonon modes originating from the significantly reduced atomic force constants and allow for achieving a comprehensive understanding of the lattice dynamics of epitaxial, strain-free interfaces.

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