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Lattice dynamics and polarization-dependent phonon damping in �-phase FeSi2 nanostructures

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Nanostructures of transition metal silicides have a wide range of possible applications and constitute fundamental building blocks of current micro- and nanoelectronics [1–3]. Among these compounds, $FeSi_2$ is particularly interesting since it is the only representative that exists in both metallic and semiconducting bulk-phase [4]. The high-temperature metallic α-phase can be stabilized at room temperature by growth of metastable, surface-stabilized nanostructures on Si surfaces. While the electronic and magnetic properties of this material are studied extensively and reveal noteworthy results [5,6], only particular thermodynamic properties have been investigated and the lattice dynamics remains unknown until now.
In this work [7], we present an experimental and theoretical study of the lattice dynamics of surface-stabilized α-phase $FeSi_2$ nanostructures epitaxially grown on the Si(111) surface, with average heights and widths ranging from 1.5 to 20 nm and 18 to 72 nm, respectively. The crystallographic orientation, surface morphology and local crystal structure of the nanostructures were investigated by reflection high-energy electron diffraction, atomic force microscopy and X-ray absorption spectroscopy. The Fe-partial phonon density of states (PDOS), obtained by nuclear inelastic scattering, exhibits a pronounced damping and broadening of the spectral features with decreasing average island height. First-principles calculations of the polarization-projected Si- and Fe-partial phonon dispersions and PDOS enable the disentanglement of the contribution of the xy- and z-polarized phonons to the experimental PDOS. Modelling of the experimental data with the {\it ab initio} results unveils an enhanced damping of the z-polarized phonons, while the xy-polarized phonons remain mostly unaffected. This phenomenon is attributed to the fact that the low-energy z-polarized phonons exhibit a stronger coupling to the low-energy surface/interface vibrational modes. The thermodynamic and elastic properties obtained from the experimental data show a pronounced size-dependent behaviour.

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