Experiment title: *Lattice dynamics of metallic and semiconducting $FeSi_2$ nanowires* (MA 3725)

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The aim of the experiment was a systematic study of the lattice dynamics in $FeSi_2$ nanostructures. For this purpose we prepared $FeSi_2$ films in the semiconducting β-phase and nanoislands and nanowires in the metastable, surface stabilized metallic γ-phase. The growth by molecular beam epitaxy and the *in situ* structural characterization with RHEED, XPS and AFM were conducted at KIT, Karlsruhe. Six samples were transported to the ESRF in a UHV transport case at a base pressure of 10^-10 mbar. On site the samples were transferred under UHV conditions to a portable ultrahigh-vacuum system designed for *in situ* X-ray scattering and spectroscopy experiments at synchrotron radiation beamlines.

Figure 1 shows three examples of spectra measured in different $FeSi_2$ nanostructures. In Fig.1 (a) the Fe-partial PDOS of a bulk-like β-phase $FeSi_2$ film measured in two orthogonal directions is compared with the related *ab initio* calculated PDOS. Except for a small shift of the main peak a very good agreement between measurement and theory is observed. Fig.1 (b) shows the phonon DOS of γ-phase $FeSi_2$ nanoislands also measured in two orthogonal directions. As expected, no vibrational anisotropy has been observed for these hemispherical nanostructures. The main features of the experimental spectrum can be reproduced by the *ab initio* calculated PDOS. However, since the lattice dynamics in surface-stabilized systems is heavily influenced by interface modes, on-going more sophisticated calculations are required to fully explain our experimental findings. In Fig.1 (c) the phonon DOS of nanowires projected along and across the wires is shown. The figure reveals a pronounced vibrational anisotropy. The low-energy mode visible across the wires is suppressed along the wires and the peak intensities at 30 meV are altered. Since the γ-phase $FeSi_2$ has a cubic symmetry, the observed differences cannot be attributed to crystal anisotropy.

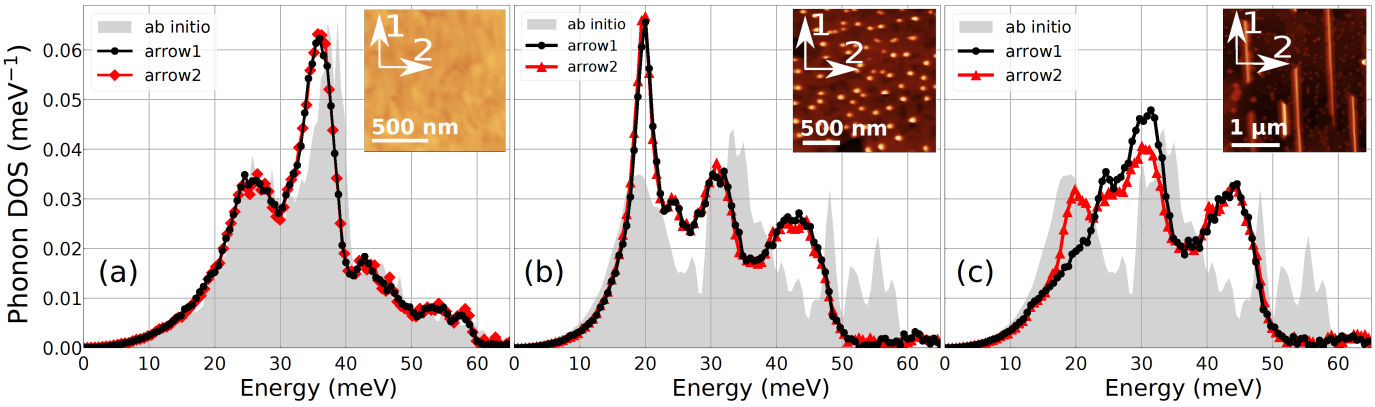

Figure 1. *The Fe-partial PDOS of (a) bulk like β-phase $FeSi_2$ film, (b) γ-phase $FeSi_2$ islands, (c) γ-phase $FeSi_2$ nanowires measured in orthogonal directions indicated by the arrows. In all graphs the phonon DOS calculated from first principles for the respective system is plotted by the shaded area. In the top right panels AFM images of the respective samples are shown.*