ESRF	Experiment title: **Vibrational dynamics of ultrathin $SmSi_2$ films, nano-islands, and nano-wires from *in-situ* nuclear inelastic scattering on ^{149}Sm**	**Experiment number**: MA-2174
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Report:

The aim of this experiment was to investigate the phonon density of states (DOS) and thermo-elastic properties of $SmSi_2$ films, nanoislands and nanowires by *in-situ* (i.e. under ultrahigh vacuum) nuclear inelastic scattering of synchrotron radiation on ^{149}Sm. The interest to investigate rare-earth silicides (RESi) stems from the fact that they self-organize in nanostructures with very low Schottky barrier height, which makes them highly attractive for applications in the near-future nanoelectronics. However, the growth of high-quality epitaxial $SmSi_2$ nanowires was not very successful. Therefore we have investigated the phonon DOS in islands, wires and films of $DySi_2$ that is the archetypal system in the field of self-organized rare-earth silicide nanostructures. The growth conditions for obtaining high quality $DySi_2$ films, nanoislands and nanowires have been optimized in the home lab at ANKA, KIT. The lattice dynamics was investigated by *in-situ* nuclear inelastic scattering on ^{161}Dy.

The experiment was performed at ID18 of the ESRF using the ultrahigh vacuum facility [1] installed in the second experimental hutch. We point out that this is the only place worldwide where thin films and nanostructures can be grown, characterized, and investigated by *in-situ* nuclear resonant scattering methods. We used the 16-bunch filling mode of the ESRF storage ring. The final energy bandwidth of 1.0 meV (at the resonance energy of 25.651 keV) was obtained using a dedicated high-resolution monochromator. The vertical beam size was reduced down to 12 μm using Kirkpatrick-Baez focussing mirror.

Dysprosium silicide samples with nominal Dy coverage of 20 nm (film), 0.26 nm (islands) and 0.1 nm (wires) were grown epitaxialy on the vicinal Si(100) substrate following an elaborated procedure [2]. The quality of the samples was proven by the reflection high energy electron diffraction (RHEED) measured after the samples growth and before the nuclear inelastic scattering experiment. Due to the significant multiphonon contribution to the measured signal at room temperature the samples were cooled down to 100 K. The energy dependences of the inelastic X-ray absorption were measured parallel and perpendicular to the vicinal steps of the Si(001) substrate in order to investigate the possible presence of vibrational anisotropy.

Figure 1 shows selected phonon DOS of the $DySi_2$ samples. The figure reveals remarkable modifications of the vibrational spectrum of $DySi_2$ as the sample morphology changes from bulk-like film towards self-organized nanoislands and nanowires. The DOS of the 20 nm sample (bulk) is characterized with a localized phonon mode around 14.0 meV, a low-energy tail and a rather sharp high energy cut-off at 16.0 meV. This vibrational behavior is characteristic for a rattling mode of an atom in a cage. In addition to the bulk-like phonon mode and the high-energy cut-off, the DOS of the 0.26 nm sample (islands) is shifted to lower energies with peak position at 13.0 meV. Further reduction of the Dy coverage to 0.1 nm (nanowires) results in significant changes of the phonon DOS. Namely, the spectrum is shifted to even lower energies with additional phonon modes at around 7.0 meV and 9.5 meV. These changes have important implications on the thermo-elastic properties of the $DySi_2$.

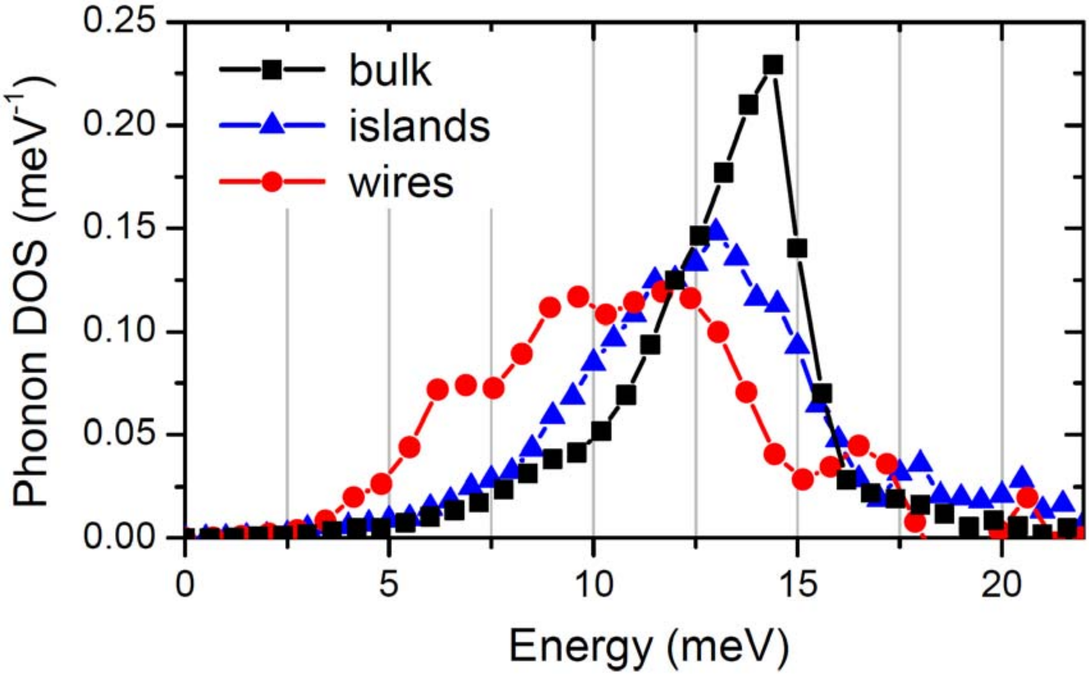

Fig. 1. *The partial Dy-projected phonon DOS of $DySi_2$ obtained from the nuclear inelastic scattering spectra measured perpendicular to the steps of the vicinal Si(001) at 100 K. A significant and systematic shift of the phonon spectrum towards lower energy (phonon softening) is clearly visible. In case of nanowires additional phonon modes are detected.*

In order to get a comprehensive understanding of the observed phonon DOS the experimental results will be compared with the results from first principles calculations that are in progress.

These results demonstrate the importance of the systematic lattice dynamics investigations in ultrathin films and nanostructures with various shapes, such as islands, clusters, and wires. This was already shown in our previous experiment on $EuSi_2$ films and nanoislands (SI-2546) [3] that is now complemented by the systematic studies of nanostructures of $DySi_2$.

References:
[1] S. Stankov et al., Rev. Scientific Instr. **79**, 045108 (2008).
[2] C. Preinesberger et al., J. Phys. D: Appl. Phys. **31**, L43–L45 (1998).
[3] S. Stankov et al., Experimental Report SI-2546.