ESRF	**Experiment title:** Lattice dynamics of GaAs/Fe_3Si core/shell nanowires	**Experiment number**: MA 5570
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Shifts: 11	Local contact(s) Sergey Yaroslavtsev	

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The aim of this proposal was to perform a systematic study of the lattice dynamics of the Fe_3Si shell in the GaAs/Fe_3Si core/shell nanowires as a function of GaAs-core diameter and Fe_3Si-shell thickness via measuring the Fe-partial phonon density of states by in situ nuclear inelastic scattering.

Report

The main aim of the experiment was a systematic *in situ* study of the lattice dynamics of the Fe_3Si shell on GaAs core nanowires (NWs) for different shell thicknesses and wires diameters. For the matter of simplification we have replaced Fe_3Si with pure Fe, which also grows epitaxially on the GaAs and the growth procedure was establish in our lab at Karlsruhe. Furthermore, in a presiding experiment performed at P01/PETRA III we investigated the Fe-partial phonon density of states (PDOS) of Fe/GaAs 2D hetersotructures with the thickness of the Fe layer of 1, 2, 3 and 36 monolayers (1 monolayer ML = 0.14 nm) in order to have the reference samples for comparison with the quasi-1D core/shell samples. The data, however, demonstrated very unusual behaviour, namely phonon hardening of the Fe-PDOS (decreasing/increasing of the low/high energy phonons) by reducing the film thickness. In order to understand this phenomenon, in our experiment we have firstly measured *in situ* the Fe-PDOS of 2D samples with thickness of the Fe layer of 2, 3 and 5 ML. In addition, a reference sample consisting of Fe crystallites deposited on the GaAs substrate was also measured. The Fe-PDOS of these samples is summarized in Figure 1(a) and shows clear features which deviate from the reference 36 ML thick Fe film. Figure 1(b) shows a comparison of the Fe-PDOS of two 2 ML thick films deposited at different temperatures obtained *in situ* with that of the *ex situ* measured sample. Figure 1(c) shows the Fe-PDOS of the 3 ML thick films measured *in situ* and *ex situ*. The last two figures indicate the presence of a clear and strong effect of the coverage of the samples, which has to be taken into account when comparing the Fe-PDOS of the core-shell NWs to that of the 2D films.

Figure 2 shows a comparison of the Fe-PDOS of the 2D film and quasi-1D core/shell NWs with a coverage of 5 ML both compared to that of 36 ML thick reference film. The Fe-PDOS show very similar features confirming that indeed the obtained PDOS of the NWs sample originates from the shell of the nanowires and there is no contribution from the Fe film parasitically deposited on the Si substrate (on which the GaAs NWs are grown). This is a proof-of-principle measurement which demonstrates that indeed it is possible to obtain the Fe-PDOS of the NWs shell with a beam size of 3x3 μm^2 used in this experiment. Figure 2

demonstrates also that at shell thickness of 5 ML there are no significant deviations from the 2D film, which is also an important information for the planning of the next measurements.

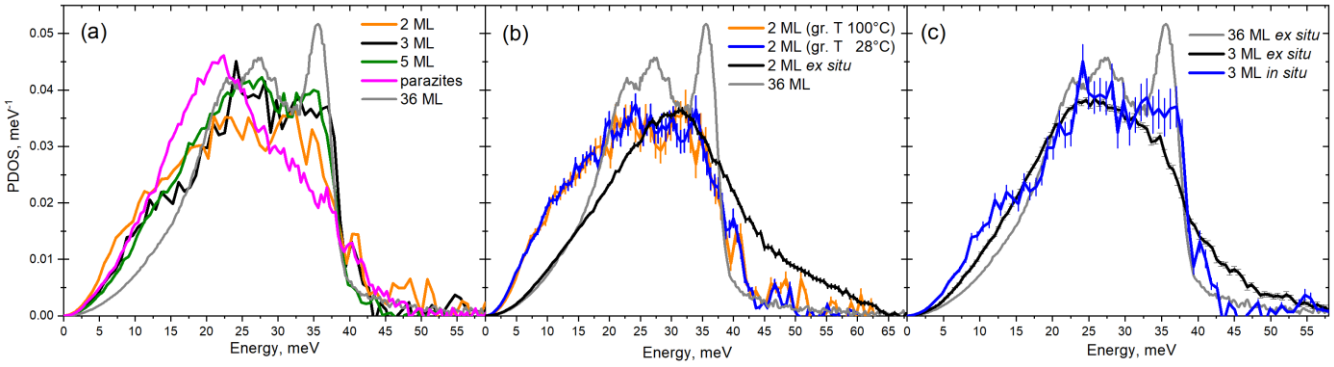

Figure 1. *(a) Fe-PDOS of all the in situ investigated 2D samples. (b) a comparison of the Fe-PDOS of Fe films with thickness of 2 ML grown at the given temperature, compared with the 2 ML sample measured ex situ (covered film); (c) a comparison of the Fe-PDOS of Fe films with a thickness of 3 ML measured in situ and ex situ. All PDOS curves are compared to that of a 36 ML thick (bulk-like) Fe film measured ex situ.*

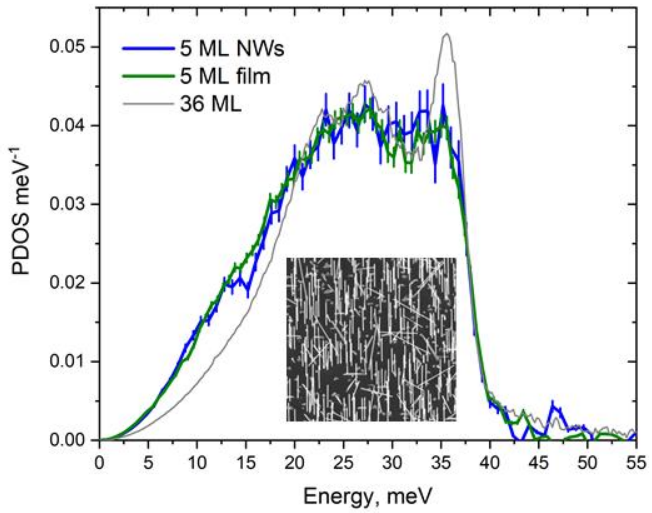

Figure 2. *A comparison of the Fe-PDOS of a 2D sample (film) and a quasi-1D sample (NWs shell) with a coverage of 5ML measured in situ. For a reference, the Fe-PDOS of a 36ML thick film is shown. The insets depicts a scanning electron microscopy (SEM) image of the investigated GaAs-core/Fe-shell nanowires.*

To summarize, with this experiment we:

1. Determined the Fe-PDOS of the 2D system Fe/GaAs for films with thicknesses of 2, 3 and 5 ML *ex situ* and *in situ*. This is an important information, which is needed in order to compare the PDOS of the Fe-shell on the GaAs-core nanowires.
2. We determined the Fe-PDOS of the Fe-shell with a thickness of 5 ML, which shows very similar features to those of the Fe film on the GaAs substrate. This is very important information because:
   (i) it demonstrates that it is possible to determine only the PDOS of the shell of the NWs without any contribution from the parasitically grown film on the Si substrate between the NWs, which is three times ticker from the shell;
   (ii) The obtained PDOS of the 5 ML Fe-shell gives an upper limit of the shell thickness, which have to be investigated, i.e. in the follow-up experiment we will measure the PDOS of the shell with a thickness of 1, 2, 3, and 4 ML both *in situ* and *ex situ*.