ESRF	**Experiment title:** Phonon dispersion in Lanthanides: Gd (and Sm, Eu, Dy)	**Experiment number:** HS 3070
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Report:

Gadolinium belongs to the group of lanthanoides and shows half filled 4f states and a 5d state with one electron. With its large absorption cross section for neutrons X-ray scattering the only possible method for this material.

Only a few measurements and model calculations exist, and those are not consistent with each other. In this experiment the aim was to determine for the first time the full set of dispersion curves of Gd and to compare with other recently measured phonons in Dy and Pu. Also, the existence of Kohn anomalies (like found in Pu) should be investigated.

Experimental Setup:

The experiment was performed at room temperature. As Gd is in the ferromagnetic state below $T_c \approx 290\,\mathrm{K}$, the sample was in or at least close to the paramagnetic state, or the magnetic moment was small.

The single crystal with the size of $2 \times 2 \times 1\,\mathrm{mm}^3$ has been purchased from MaTecK GmbH, Jülich, Germany, and was preoriented with an accuracy of $< 0.01°$ and polished on one side with an accuracy of $< 0.03\,\mu\mathrm{m}$. The three sides of the crystal have the orientation $[10\bar{1}0]$, $[11\bar{2}0]$, and [0001]. The experiment has been performed in reflection geometry.

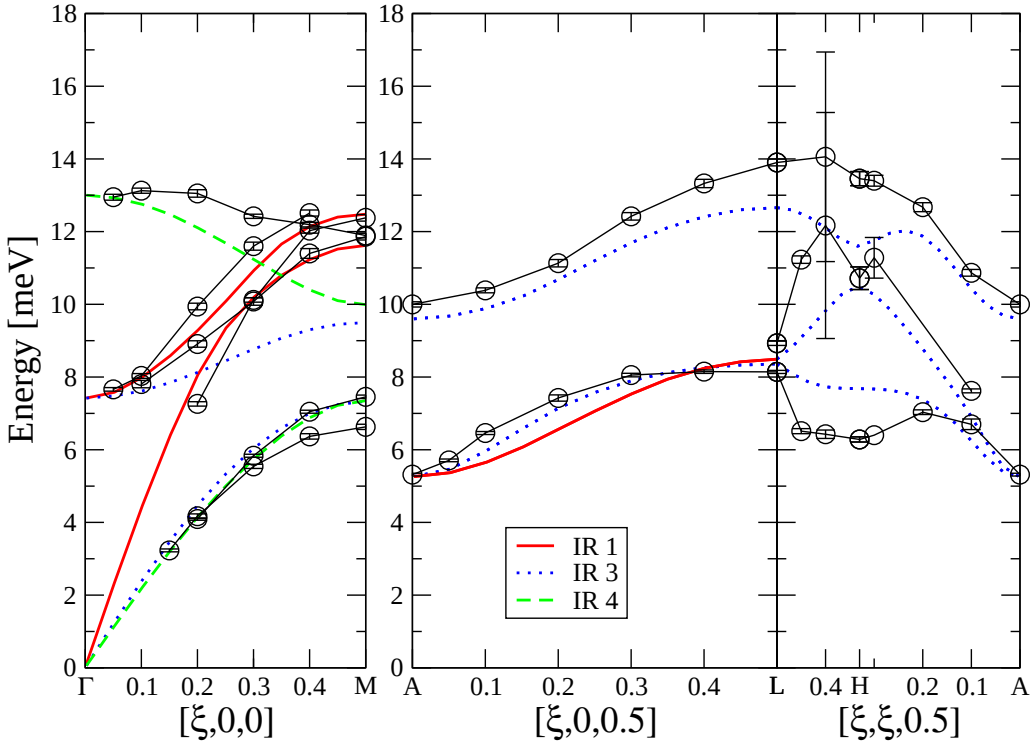
The experiment was done with three different crystal orientations: The first orientation was with the $[1\bar{1}00]$ scattering plane with phonons investigated in the directions Γ-K-M, Γ-A, A-H-L, and L-M. By a 30°-rotation of the crystal the second scattering plane was $[01\bar{1}0]$ with measurements along Γ-M and L-A. Another 90°-rotation yielded the third [0001] scattering plane, and data were taken along Γ-K-M and Γ-M with polarisations different from the first two orientations.

Results:

Along Γ-K-M and Γ-M there are six branches with three different representations. In the third orientation only four branches (two representations, IR 1 and IR 3) were visible in these directions (see figure below).

M-L shows also no degeneracies, but in our geometry we were able to see only four branches out of six. Γ-A has 4 branches, all visible, consisting of four representations, where two were doubly degenerate. Only here can one distinguish between longitudinal and transverse polarisations, all others are of mixed character. Along A-H-L and L-A there are only three branches which are doubly degenerate. Along A-H-L all branches are of the same representation and were all visible, and along L-A two doubly degenerate branches with the same representation were visible, see figure below.

Simultaneous numerical calculations assisted the effective use of beam time. *Ab initio* calculations for Gd turn out to be more time consuming than anticipated and are still running. In the mean time model calculations of phonon properties and scattering intensities were performed. The figure below shows a selected set of preliminary results of the experimental data points for the symmetry directions Γ-M, A-L, and L-H-A together with dispersion curves from a simple model with interaction between nearest and next nearest neighbours.



Phonon dispersion of Gd from measurement and model calculation in the symmetry directions Γ*-M, A-L, L-H-A.*

Contrary to other model calculations or models with only first neighbour interaction we found in the experiment a clear splitting of the two lowest modes at the L-point. At present we speculate about a Kohn anomaly at or near the H-point $[\frac{1}{3}\frac{1}{3}\frac{\overline{2}}{3}\frac{1}{2}]$, see the dip in the middle experimental curve in the right panel of the figure.