ESRF	**Experiment title:** Delocalisation of the 4f-electrons of Sm metal at high pressure	**Experiment number**: HE1594
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Report:

The experiment HE1594 was aimed at continuing the investigations started with HE1377 on the effect of external pressure on the stability of the 4f-magnetism in Sm metal by using Nuclear Forward Scattering (NFS) of synchrotron radiation. The measurements have been carried out in 16-bunch mode at beamline ID22N. A new high resolution monochromator has been designed for the energy of the ^{149}Sm resonance (22.494 keV). This delivers a flux of 8×10^7 photons/s in a bandwidth of ~0.9 meV and is therefore perfectly suited for high-pressure NFS and for Nuclear Inelastic Scattering studies. The beam was vertically collimated by using a Be compound refractive lens and focused horizontally to a size of ~150 μm, matching the size of the sample in the Diamond Anvil Cell (DAC). The sample was a Sm metal foil, enriched to 97% in ^{149}Sm. The typical counting rates for the sample in the DAC were 0.5-5 counts per second, allowing us to measure a single spectrum in 20-90 minutes. For this beamtime it has been possible to measure ~70 NFS spectra in the pressure range 22-46 GPa. X-ray diffraction patterns of the Sm foil have been measured at all pressures and at low temperatures to follow all structural phase transitions.
Fig. 1 shows the NFS spectra measured at 3 K and various pressures. At ambient pressure and at p=3.4 GPa, Sm metal has the Sm-type hexagonal structure, whose unit cell consists of nine planes stacked along the c-axis. In six of these planes, the Sm atoms have a hexago-

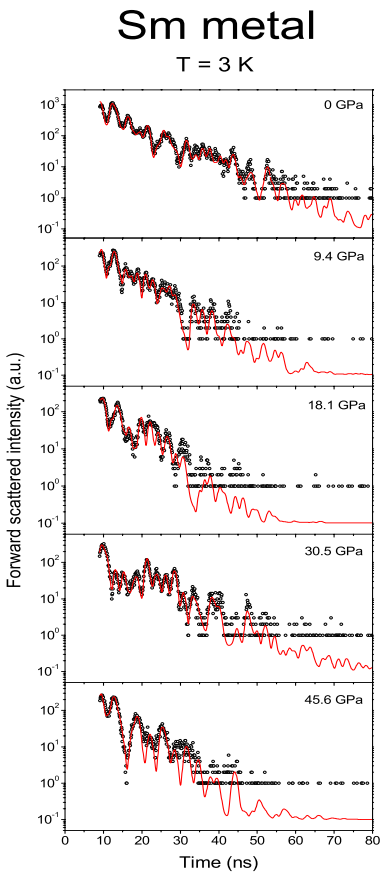

Figure 1 – NFS spectra of Sm metal at 3 K and different pressures. The circles are the experimental data points, while the continuous lines are the fits.

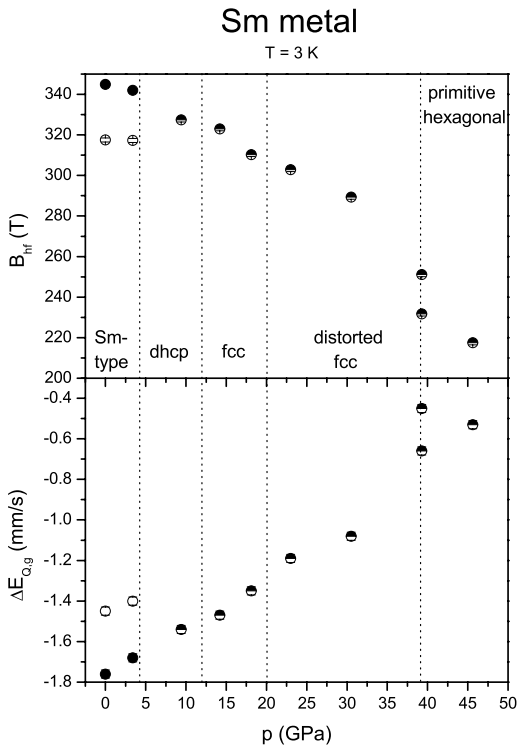

Figure 2 – Pressure dependence of the hyperfine magnetic field (B_{hf}) and of the quadrupole interaction ($\Delta E_{Q,g}$) at 3 K. The filled circles refer to the hexagonal sites and the empty to the cubic sites in the Sm-type structure while the half filled circles refer to the single in the other structures.

nal coordination, while in the remaining three the coordination is cubic. The NFS spectra are best fitted if one assumes at the cubic sites slightly reduced hyperfine interactions with respect to those at the hexagonal sites. The magnetic hyperfine field of the hexagonal sites at ambient pressure has approximately the value of the Sm^{3+} free ion. It decreases when pressure is increased to 3.4 GPa, as shown In Fig. 2. The magnitude of the electric quadrupole interaction follows the same behaviour. When pressure is increased further, above 4 GPa (at room temperature) the structure changes to *dhcp* and the ratio of hexagonal and cubic sites becomes 1:1. The NFS spectra show that in this structure both types of sites have the same hyperfine interactions, probably because of the stronger interaction between planes of different coordination. Further increases in pressure induce the successive structural transitions *dhcp-fcc-distorted fcc-primitive hexagonal*. For all structures a single Sm site is observed (at 39.3 GPa there is a coexistence of the two crystallographic phases *distorted fcc-primitive hexagonal*). The magnitudes of the hyperfine magnetic field and of the quadrupole interaction decrease as pressure increases, owing to the possible interplay of crystal field effects and conduction electron contributions. The *primitive hexagonal* phase shows a reduced magnetic hyperfine field, possibly because of the start of the delocalization of the 4f electrons, which are supposed to be involved in the chemical bonding in this phase [see Y. C. Zhao et al., Phys. Rev. B 50, 6603 (1994)]