ESRF	**Experiment title: High pressure study of the magnetic semiconductors GdX (X=As, Sb, Bi): search for new structural phases in the pressure range 20-50 GPa**	**Experiment number**: HS1206
Beamline: ID30	**Date of experiment**: from: 28/02/00 to: 03/02/00	**Date of report**: 01/09/00
Shifts: 9	**Local contact(s)**: S. Carlson	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Goncharenko Igor*, Laboratoire Leon Brillouin, CEA-CNRS, Saclay, France

Mirebeau Isabelle*, Laboratoire Leon Brillouin

Ochiai Akira*, Niigata Univeristy, Niigata, Japan

Report:

The EuX (X=O,S,Se,Te) and GdX (X=N,P,As,Sb,Bi) have been considered for decades as "textbook systems" to study magnetic interactions in semiconductros (semimentals) with localised magnetic shells. At the resent years we have performed an extensive study of the magnetic properties of the EuX and GdX families under pressure, using recently developed technique for magnetic neutron diffraction studies in the 50 GPa – pressure range [1]. From our neutron results we suggest a possibility of structural transitions in the GdX compounds in the pressure range 20 – 50 GPa, accompanied by drastic changes in their magnetic structures. It seemed to be reasonable to combine our neutron data (obtained at the LLB) with X-ray ones in order to get full information about magnetic and crystal structure of the GdX compounds under pressure. ESRF provided excellent conditions for the X-ray part of the study.

We have performed high pressure studies of the GdAs, GdSb and GdBi in the pressure range 0-50 GPa using the beamline ID30. We discovered new pressure induced structural phases. In the GdAs, the initial NaCl-like packing remains stable up to 40 GPa. In the pressure range 40 – 47 GPa we observed a structural transition to a tetragonal phase (distorted CsCl –type, see Fig.1). The same transition has been found in the GdSb in the pressure range 23 – 28 GPa. In both cases we observed intermediate phases near the critical pressures. In the GdBi we have found several polimorphic phases in the pressure range 0 – 20 GPa. At the low pressures, besides the well-known cubic phase (NaCl) we have found a rhombohedral phase (distorted NaCl). In the pressure range 9-23 GPa all the NaCl-like phases (cubic or rhombohedral) transform to the cubic CsCl-like phase (see Fig.2).

Our results should be compared with those obtained for the EuX compounds. In the EuX compounds, the NaCl –like structure transform to the CsCl-like structure in the pressure range 10-50 GPa [2]. We conclude that the transition NaCl-like – CsCl-like is the general trend under very high pressures in both families. Previous X-ray measurement did not detect any distorted/intermediate phases in the EuX family [4]. In order to be sure that the intermediate phases were not missed in the previous studies, we have measured under pressure EuS, EuSe and EuTe. The high-quality X-ray data confirmed that in the EuX compounds the phase transition NaCl-CsCl occurs abruptly, without any intermediate phases. Finally, the two families show substantial difference under high pressures. In the GdX compounds, the crystal structure seems to be more "soft" and than in the EuX ones, the structural transitions occur more smoothly through distorted intermediate phases. In contrast to the EuX-family the pressure behaviour of the GdX-family can not be explained in a framework of the simple ionic model.

The obtained results are crucial for understanding of the magnetic properties of the EuX and GdX compounds under pressure. The discovered structural transitions help to understand evolution of the magnetic structures, for example a two-step magnetic transition in the GdAs in the pressure range 40-50 GPa (found by neutron diffraction). The "smooth" (multi-step) variation of the crystal structure between the NaCl and CsCl-pases i the GdX compounds gives a unique opportunity to understand the relationship between the crystal structure and magnetic interactions. At the present, new neutron diffraction measurements are in progress in order characterize magnetic order in the discovered polymorphic phases of the GdBi. After complete characterisation of the magnetic and crystal structure of the GdX compounds in the pressure range 0 –50 GPa we intend to extend the X-ray/neutron study in the pressure range above 50 GPa.

In conclusion, we discovered new structural phases in the GdAs, GdSb and GdBi under pressure. The combined X-ray (ESRF) and neutron (LLB) study allows at the first time to characterise fully long-range magnetic order and crystal structure in the 50 GPa pressure range.

[1] I. N. Goncharenko, I. Mirebeau, Phys. Rev. Lett. 80 (1998), 1082 Europhys. Lett. 37 (1997), 633; Rev. High Pressure Sci. Technol. 7 (1998) 475.

[2] A. Jayaraman, K. Singh, A. Chaterjee and S.Devi, Phys. Rev. B9 (1974) 2513

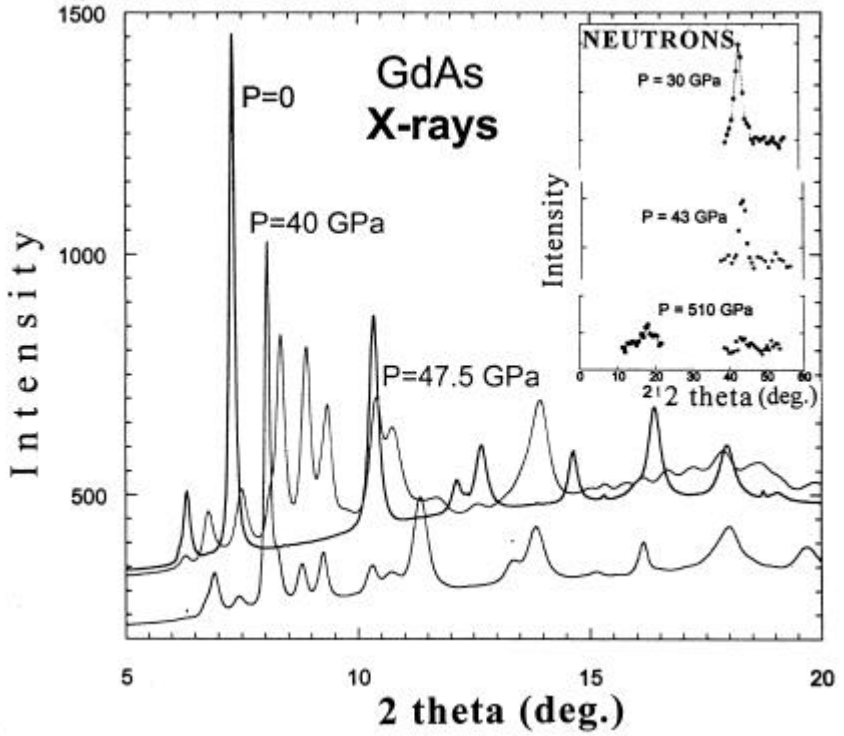

Fig.1 X-ray and neutron diffraction (on the insert) diffraction data for the GdAs

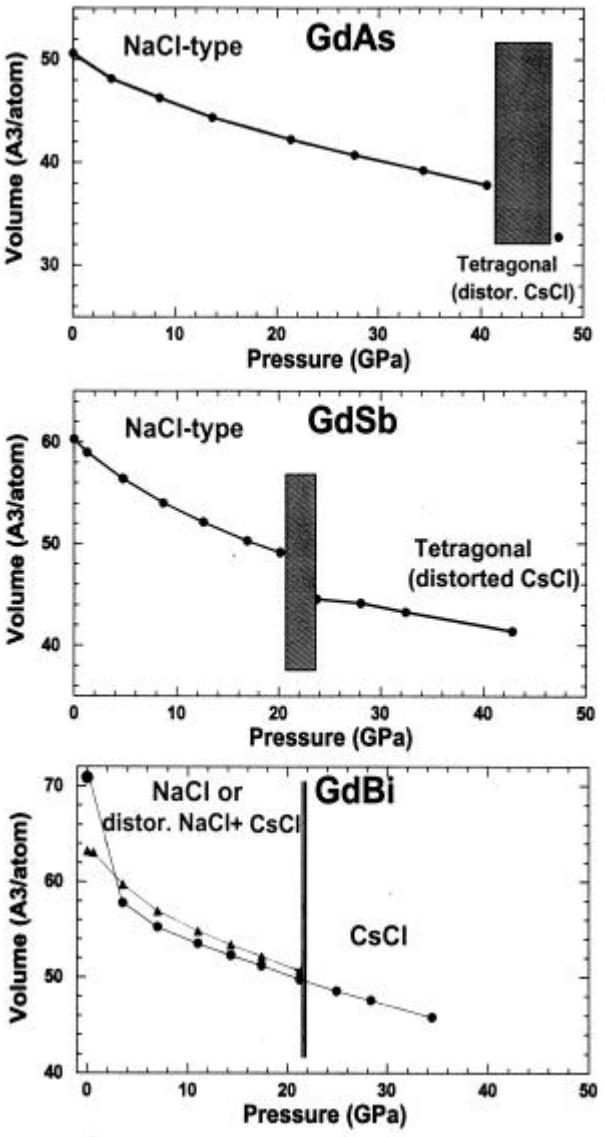

Fig.2 Equations of state and structural transitions in the GdX compounds. The grey areas indicate the transition regions.