ESRF	**Experiment title:** Study of intralayer and interlayer compresibilities of GaTe by linearly polarised EXAFS on single crystals	**Experiment number:** CH-364
Beamline: *ID24*	**Date of experiment:** from: 20/9/97 to: 25/9/97	**Date of report:** 9/7/98
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Report:

Introduction

The monoclinic (B2/m) low pressure modification of GaTe [l] is a layered semiconductor with a band gap of 1.68 eV in ambient conditions. Opposite to hexagonal or rhombohedral layered semiconductors (GaSe, InSe), GaTe layers are anisotropic due to the fact that one third of the Ga-Ga bonds are nearly in the layer plane. The structure of GaTe has been studied under pressure by means of X-ray diffraction [2]. A first order high pressure transition to a high-pressure NaCl type polymorph was found. For decreasing pressures, the NaCl phase is observed until 3.2 GPa, pressure at which the material becomes amorphous.

EXAFS with polarised light on monocrystals can provide useful information about the anisotropy of GaTe layers and its behaviour under pressure.

Experimental

GaTe needles were grown by vapor phase transport. The needles grow in the direction perpendicular to the in-plane Ga-Ga bonds and are very easily cut and oriented, as they have mirror-like faces parallel to the layers and edges parallel to the c-axis. The sample size was $100x100x50\ \mu m^3$. For the high pressure experiment a membrane diamond anvil cell was used, with silicone oil as pressure transmitting medium and ruby as pressure gauge. The polarization of the X-rays with respect to the sample anisotropy axis was changed by turning the cell around its axis, after careful selection of the cell positions in which any difraction peak from the diamonds was observed. EXAFS measurements were carried out at the Ga K-edge (10.368 keV). The detector calibration was frequently checked along the experiment with a reference Gas sample, whose EXAFS spectrum had been previously measured in the classic configuration, at ID29.

Results and discussion

Figure 1 shows the EXAFS spectra at the Ga K-edge, at different pressures and for X-ray polarisation perpendicular and parallel to the GaTe c-axis. The transition to the NaCl phase at 10 GPa is apparent in this series from the change of the shape and the disappearence of the anisotropy. Figure 2 shows the result of the analisis. Both the Ga-Te and the in-plane Ga-Ga bond lengths could be determined as a function of pressure, in spite of the small amplitude of the latter. Our measurements show that both the Ga-Ga distance and the Ga-Te are much less compressible that what could be inferred from the bulk compressibility, as deduced from X-ray diffraction studies. The difference between the two results can be only explained through the variation of Ga-Ga-Te and Te-Ga-Te angles. In the NaCl phase both the first and second neighbor distances could be determined. In that phase, local and bulk compressibihties coincide.

References

1 .M. Julien-Pouzol,S. Jaulmes,M. Guittard, Alapini F. Acta Cryst., B35, 2848-5 1 (1979).
2.U. Schwarz, K. Syassen,R. Kniep.Journal of Alloys and Compounds, 224,212-6 (1995).

(These results will be presented at the 8th International Conference on High Pressure Semiconductor Physics, to be held in Thesaloniki, Greece, 9-13th August 1998)

Figure 1

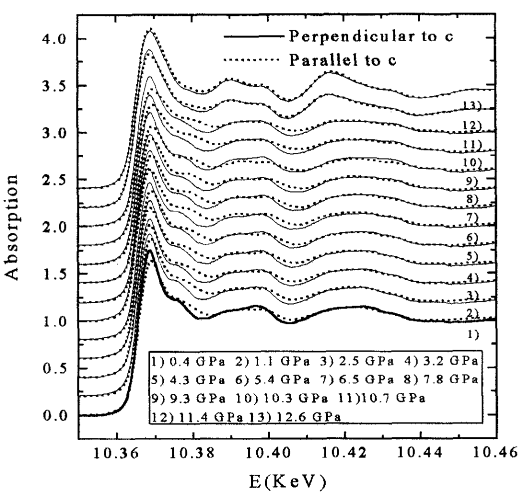
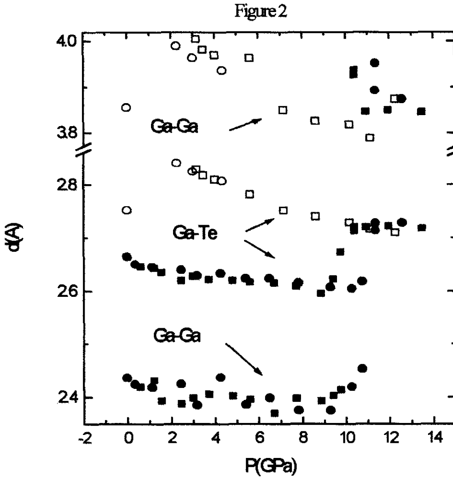


Figure2



Suplementary comments to the report on the experiment CH-364, "Study of intralayer and interlayer compressibilities of GaTe by linearly polarised EXAFS on single crystals".

These comments essentially refer to the use of the beam time allocated to the experiment.

- The first day was spent in the implementation of the spectroscopic system to measure the pressure inside the diamond anvil cell. That system was borrowed from the high pressure line. The implementation of the system included the programmation of several macros to move the microscopic optical system and the diamond cell holder between the EXAFS measurement position and the pressure measurement position. This movement must be computer-controlled in order to guarantee the reproducibility of the positions and avoid the dammage of the capillary of membrane diamond- cell . Along the experiments, those movements took more time than the EXAFS measurements at each pressure.

- The preparation of the EXAFS experiment also included a careful selection of the cell orientation in order to avoid the appearence of diamond diffraction related structures in the transmitted beam. As each measurement had to be done at two different orientations, finding those orientations took also a long time.

- We were able to perform two complete experiments with two different GaTe samples, from ambient pressure to 15 GPa, at the Ga K-edge. Figure 2 in the report includes the results of the interpretation of both series of experiments.

- Along the last night we carried out a suplementary experiment with an InSe sample, at the Se K-edge (12.658 KeV), from ambient pressure to 14 GPa. At this photon energy range the number of diamond diffraction peaks is much higher than in the Ga K-edge range. It was impossible to find an orientation with no diffraction peaks in the EXAFS range. Consequently, each EXAFS spectrum had to be taken at different cell orientations in order to cover a wide photon energy interval, by superposing spectra taken at different orientations (it must be outlined that this technique is possible because, opposite to GaTe, InSe layers are isotropic). The reconstruction of the EXAFS spectra is being more laborious, but it will certainly yield very useful results. Once these results are interpreted, we will send you a suplementary abstract.