PRESSURE INDUCED PHASES TRANSITIONS IN GaP: AN X RAY ABSORPTION SPECTROSCOPY INVESTIGATION

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PRESSURE INDUCED PHASES TRANSITIONS IN GaP: AN X RAY ABSORPTION SPECTROSCOPY INVESTIGATION

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Under high pressure, GaP exhibits a phase transition near 25 GPa, determined by optical measurements (1,2) and X ray diffraction (3,4). When pressure is released, according to X ray diffraction, the transition is reversible, although the diffraction peaks are weaker. But the sample remains black and optical properties of the initial phase are no longer observed.
We have performed an X ray absorption spectroscopy experiment, at the Ga K edge, on GaP up to 36 GPa, using the energy dispersive mode(5).
Finely powdered GaP has been loaded in a classical diamond anvil cell with silicone oil as pressure transmitting medium. A ruby chip was added to measure the pressure. The sample size was about 250 μm in diameter and 30 μm in thickness. Due to the optimized shape of the Si crystal(6), the energy range has been extended up to 400 eV .
The zincblende phase of GaP remains stable up to 23 GPa. In figure 1, at 11.5 GPa, a shift of the XANES to high energy is observed. Such a behaviour is consistent with a decrease of the Ga-P bond length (fig 2). The variation of the Ga-P distance has been determined using the classical EXAFS fitting procedure. The backscattering amplitude and the phase shift was obtained from the zero pressure data. The results have been fitted to a Murnaghan equation of state with B=88.1 GPa and B'=4.5 . The value of the bulk modulus is in good agreement with ultrasonic data (B=87.5 GPa).
At 26 GPa, the spectrum is perturbated by the mixing of two phases. At 36 GPa, the transition is complete and the near edge spectrum is different from

the low pressure one (fig1). In figure 2,c, an increase of the first neighbour distance is observed, indicating a change in the neighbour configuration. A two shells adjustement, with 4 P and 2 Ga gives 2.41 A and 2.44 A for Ga-P and Ga-Ga distances respectively. These results are in good agreement with the β tin structure proposed(3,4) for the GaP high pressure phase.
When pressure is released, the near edge spectrum differs from both high and low pressure spectra(fig1). It looks like amorphous GaP. The lack of second neighbours in figure 2,d, leads to the same conclusion: a large amount of the sample is amorphous. The existence of a zincblende diffraction pattern(2) indicates that a small part of the sample reverts to the initial phase. A partial amorphisation accounts for the weakening of the diffracted lines and the change in optical properties.

1 J.P.Pinceaux, J.M.Besson, A.Rimsky and G.Weil, in High Pressure Science and Technology vol 1, ed B.Vodar and P.Marteau, Pergamon press,Oxford (1980) p 241
2) C.Jauberthie-Carillon and C.Guillemin unpublished
3)M.Baublitz and A.L.Ruoff, J of Appl. Phys. 53, 6179 (1982)
4)J.Z. Hu, D.R.Black and I.L.Spain, Sol. Stat. Comm. 51, 285 (1984)
5) E.Dartyge, C.Depautex, J.M.Dubuisson, A.Fontaine, A.Jucha and G.Tourillon, N.I.M. A246, 452 (1986)
6) H.Tolentino, E.Dartyge, A.Fontaine and G.Tourillon , J. Appl. Cryst. 21, 15 (1988)

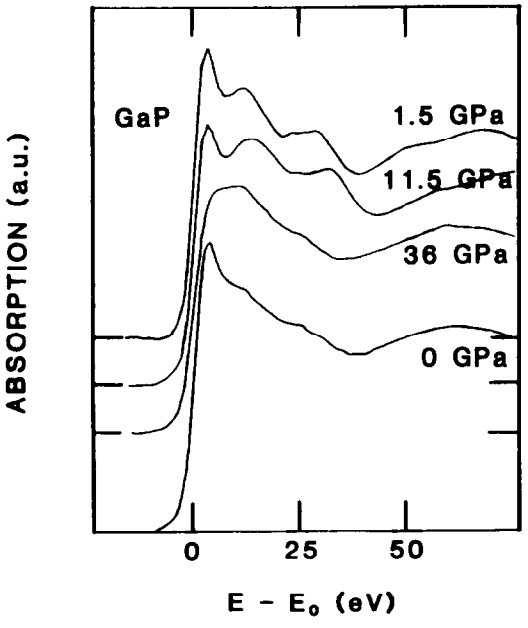

fig1:XANES of GaP at different pressures

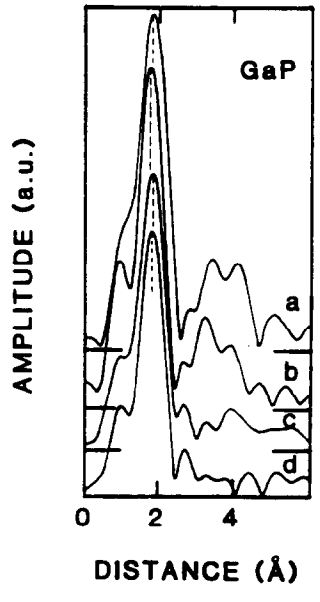

fig2:Fourier transform of GaP EXAFS
a)1.2 GPa, b)11.5 GPa, c)36 GPa
d)0 GPa after releasing pressure