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HIGH-PRESSURE DIFFRACTION STUDY OF $Ga_{1-x}Al_xAs$

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The $Ga_{1-x}Al_xAs$ sample of $x = 0.5$ was prepared from a high quality single crystal grown by electroepitaxy on GaAs. The high-pressure diffraction experiments were performed using a diamond anvil cell and a germanium solid state detector. The zinc-blende phase is stable up to about 17.5 GPa on uploading. A high-pressure phase manifests itself at about 17 GPa, a complete phase change occurs at 18.7 GPa. On downloading, the zinc-blende phase reappears at about 10 GPa. The powder pattern of the high-pressure phase shows some similarities with the GaAs high pressure phases.

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1. Introduction

High-pressure phase transitions in binary III–V compounds are subject of extensive X-ray diffraction studies (see, e.g., [1–7]). Rapid advances in such investigations are connected with the progress in the availability and quality of synchrotron radiation sources and data collection systems. To the best of our knowledge, there had been no reported experimental work on phase transitions in III–V solid solutions. An example of such solution is $Ga_{1-x}Al_xAs$ being an important semiconductor material with numerous applications. The high-pressure transitions are different for GaAs and AlAs. Therefore, it is interesting to determine whether and in what range the solid solution conserves the high-pressure structure types of its binary end members. The zinc-blende GaAs transforms to the orthorhombic GaAs-II type [2] (see also data of Ref. [1]). The transition pressure has been concluded to be $12(\pm 1.5)$ GPa [8]. This high-pressure structure type is specific for GaAs. With a further increase in pressure, there are other phase transitions in GaAs [2]. The zinc-blende AlAs transforms to the hexagonal NiAs type. This transition has been found experimentally [3] (transition pressure 7 ± 5 GPa) and supported by *ab initio* calculations [6]. The NiAs type is known for another III–V high-pressure phase, AlP [9] and for a larger number of II–VI compounds [6].

2. Experimental

The $Ga_{1-x}Al_xAs$ sample, with $x = 0.5$, was prepared from a high quality single crystal grown by electroepitaxy on a (100) oriented GaAs substrate. The substrate was dissolved using preferential etching and then the finely ground crystal was mixed with NaCl treated as a pressure transmitting medium and as a pressure marker. The experiments were performed at HASYLAB on F3 line in energy-dispersive mode using a diamond anvil cell and a germanium solid state detector. The applied diffraction angle was $\theta = 5.2374°$.

3. Results

The pressure–volume dependence (cf. Fig. 1) allowed us to obtain the bulk modulus of the zinc-blende phase which is stable up to about 17.5 GPa on uploading. The bulk modulus value and its first derivative (72.5 GPa and 4.2, respectively), calculated in this work by fitting the Birch–Murnaghan equation [10], are in reasonable agreement with interpolated literature data [11] for $Ga_{1-x}Al_xAs$ (Table).

New peaks belonging to a high-pressure phase manifest themselves at about 17 GPa. Further uploading leads to a complete phase change observed at 18.7 GPa, where the zinc-blende-type peaks disappear. Downloading starting from 18.7 GPa causes first an enhancement of some weak peaks already visible at 18.7 GPa. The zinc-blende phase reappears at about 10 GPa, so the transition may be concluded to occur at about 13.5 GPa with hysteresis ranging from 10 to 17 GPa. The transition pressure is closer to the GaAs case while the hysteresis is intermediate

TABLE

The bulk modulus value for $Ga_{1-x}Al_xAs$, $x = 0.5$, calculated by fitting the Birch–Murnaghan equation compared to the literature values for zinc-blende-type $Ga_{1-x}Al_xAs$, GaAs and AlAs. Starred is the value obtained from the linear dependence $B_0(x)$ [11].

Composition	Bulk modulus B_0 [GPa]	First pressure derivative of the bulk modulus dB_0/dp	Reference
GaAs	75.5		[11, 12]
		4.49	[12]
$Ga_{0.5}Al_{0.5}As$	76.8*		[11]
	72.5	4.2	this work
AlAs	78.1		[11]
	74(4)†	5(1)†	derived in [6] from data of [4]
	74.2	4.3	average of theoretical values collected in [6]

† numbers in parentheses refer to the error values.

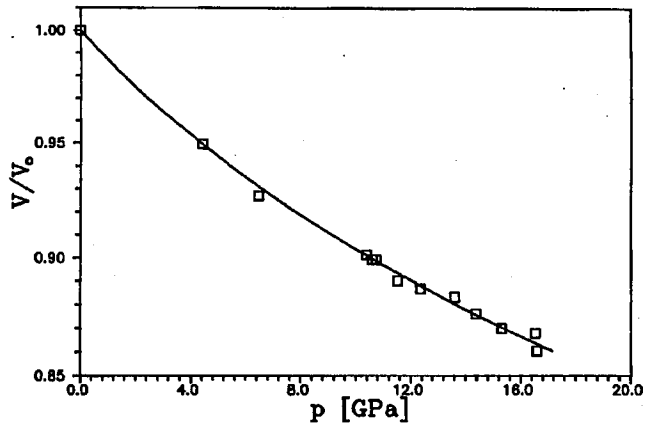

Fig. 1. Compression of zinc-blende type $Ga_{0.5}Al_{0.5}As$.

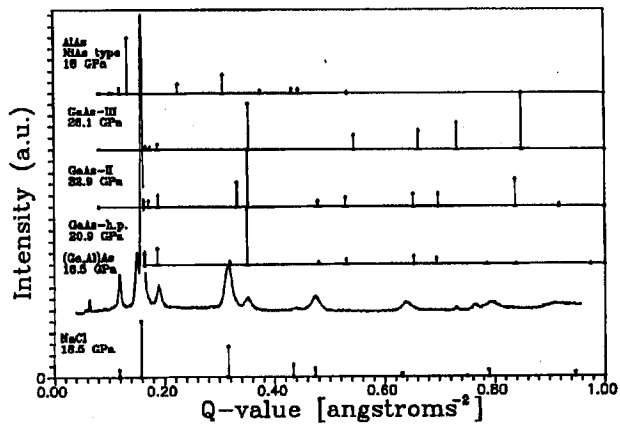

Fig. 2. A comparison of the high-pressure powder pattern for $Ga_{0.5}Al_{0.5}As$ with literature data for GaAs and AlAs. The following powder patterns are included: in the form of bars representing peak positions and intensities: AlAs of NiAs type at 18 GPa [3], GaAs-III at 28.1 GPa [2], GaAs-II at 22.9 GPa [2], high-pressure GaAs at 20.9 GPa [1]; powder pattern of $Ga_{0.5}Al_{0.5}As$ obtained in this work at 18.7 GPa; peak positions and intensities for NaCl pressure marker; the positions are derived from the NaCl equation of state, the intensities are those of the ICDD standard at ambient conditions.

between GaAs and AlAs cases. The powder diagram of the high-pressure phase is compared with the literature data for binary GaAs and AlAs in Fig. 2. It shows some similarities with GaAs literature data being markedly different from the NiAs type observed for AlAs. A possible overlap with NaCl lines makes the analysis of the new high-pressure phase difficult and indicates that using another pressure marker should be considered in more systematic investigations.

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