X-ray diffraction study on pressure-induced phase transformations and the equation of state of $ZnGa_2Te_4$

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We report on high-pressure x-ray diffraction measurements up to 19.8 GPa in zinc digallium telluride ($ZnGa_2Te_4$) at room temperature. An irreversible structural phase transition takes place at pressures above 12.1 GPa and upon decompression a third polymorph of $ZnGa_2Te_4$ was recovered as a metastable phase at pressures below 2.9 GPa. Rietveld refinements were carried out for the three detected polymorphs, being their possible crystal structures reported. The axial compressibilities for the low-pressure phase of $ZnGa_2Te_4$ have been determined as well as the equation of state of the low- and high-pressure phases. The reported results are compared with those available in the literature for related compounds. Pressure-induced coordination changes and transition mechanisms are also discussed. © *2013 AIP Publishing LLC*. [http://dx.doi.org/10.1063/1.4851735]

I. INTRODUCTION

Defect-chalcopyrite (DC) and defect-stannite (DS) compounds are members of the adamantine-type AB_2X_4 family of semiconductors. These materials are currently being investigated due to their diversity of applications which include optoelectronics, non-linear optics, and electro-optics among others.[1] Zinc digallium telluride ($ZnGa_2Te_4$) is part of this family of compounds. It has been proposed as a promising material for developing phase-change memory devices.[2] To develop these potential applications, a correct determination of the electronic properties of $ZnGa_2Te_4$ is needed, for which a precise knowledge of its crystal structure is fundamental. This structure has been studied by x-ray diffraction (XRD)[3] and *ab initio* calculations.[4] According to previous experiments, $ZnGa_2Te_4$ crystallizes in the tetragonal DC structure (space group $I\bar{4}$), however, its structure has not been fully refined and its yet under debate being also the DS structure a good candidate for it (space group $I\bar{4}2m$).[5]

High-pressure (HP) structural studies on AB_2X_4 compounds have received increasing attention in the last years. Among other techniques, they have been studied by XRD, being several pressure-induced transitions reported.[6–15] The reversibility of these transitions is subject of dispute. In some cases, it has been found that the transitions are not reversible, being metastable polymorphs recovered at ambient conditions after decompression. These polymorphs have a smaller electronic band gap than the ambient-pressure stable polymorph,[16] opening the door to novel applications for AB_2X_4 semiconductors. In contrast with other AB_2X_4 compounds, only few works have been devoted to the study of the structural properties of $ZnGa_2Te_4$[3,4] and no records of HP studies can be found in the literature. Here, we report room-temperature (RT) synchrotron HP XRD measurements up to 19.8 GPa to study into detail the structural properties of the low-pressure phase of $ZnGa_2Te_4$ and the possible occurrence of structural phase transitions. The RT equation of state (EOS) of the different polymorphs found in $ZnGa_2Te_4$ will be presented. Technical aspects of the experiments are described in Sec. II. Results are presented and discussed in Sec. III and conclusions are summarized in Sec. IV.

II. EXPERIMENTAL DETAILS

Single crystals of $ZnGa_2Te_4$ were grown by chemical vapor method using iodine as a transport agent.[17] The as-grown crystals of uniform dark-red color represent triangular prisms with mirror-like surfaces. Their chemical composition was verified by energy-dispersive x-ray analysis with a Phillips XL-30 scanning electron microscope. No impurities have been detected and the determined stoichiometry of the crystals corresponds to pure $ZnGa_2Te_4$ with a precision of 0.2%. Angle-dispersive XRD experiments were carried out at RT under pressure up to 19.8 GPa using a diamond-anvil cell (DAC) at Sector 16-IDB of the HPCAT, at the Advanced Photon Source (APS). Measurements were also carried out on decompression. Experiments were performed with an incident monochromatic wavelength (0.3681 Å). The sample used was a 10-μm thick pre-pressed pellet prepared using a finely ground powder obtained from the as grown single crystals. The pellet was loaded in a

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