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High-pressure study of the structural and elastic properties of defect-chalcopyrite $HgGa_2Se_4$

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In this work, we focus on the study of the structural and elastic properties of mercury digallium selenide ($HgGa_2Se_4$) which belongs to the family of AB_2X_4 ordered-vacancy compounds with tetragonal defect chalcopyrite structure. We have carried out high-pressure x-ray diffraction measurements up to 13.2 GPa. Our measurements have been complemented and compared with total-energy *ab initio* calculations. The equation of state and the axial compressibilities for the low-pressure phase of $HgGa_2Se_4$ have been experimentally and theoretically determined and compared to other related ordered-vacancy compounds. The theoretical cation-anion and vacancy-anion distances in $HgGa_2Se_4$ have been determined. The internal distance compressibility in $HgGa_2Se_4$ has been compared with those that occur in binary HgSe and $\varepsilon-$GaSe compounds. It has been found that the Hg-Se and Ga-Se bonds behave in a similar way in the three compounds. It has also been found that bulk compressibility of the compounds decreases following the sequence "ε-GaSe > $HgGa_2Se_4$ > HgSe." Finally, we have studied the pressure dependence of the theoretical elastic constants and elastic moduli of $HgGa_2Se_4$. Our calculations report that the low-pressure phase of $HgGa_2Se_4$ becomes mechanically unstable above 13.3 GPa. © *2013 American Institute of Physics*. [http://dx.doi.org/10.1063/1.4792495]

I. INTRODUCTION

Mercury digallium selenide ($HgGa_2Se_4$) is one of the less studied adamantine-type $A^{II}B_2^{III}X_4^{VI}$ ordered-vacancy compounds (OVCs) which crystallizes in the tetragonal defect-chalcopyrite (DC) structure with space group (S.G.) I-4, Z = 2. OVCs are tetrahedrally coordinated semiconductors, which are derived from the diamond and the zincblende or sphalerite (F-43 m) structures. They have a vacant cationic site in an ordered and stoichiometric fashion, i.e., a stoichiometric vacancy is located at a fixed Wyckoff position in the unit cell.[1] The presence of vacancies in OVCs results in a complex physics for these compounds.

OVCs are important materials to understand the role played by vacancies in the physical and chemical properties of solids because they constitute a bridge between perfect and defect materials. Besides, they are interesting materials to study order-disorder phase transitions occurring in tetrahedral semiconductors. A common trend in all adamantine OVCs is that they have several non-equivalent tetrahedrally coordinated cations resulting in a distortion of the crystal lattice from the cubic symmetry. The lack of cubic symmetry provides special properties to OVCs with important applications in optoelectronics, solar cells, and non-linear optics.[1–4] These semiconductors are of interest as infrared-transmitting window materials among other applications. They are also applied in nonlinear optical devices and in narrow-band optical filters. In addition, OVCs are promising optoelectronic materials due to their high values of nonlinear susceptibility, optical activity, intense luminescence, and high photosensitivity.[2] They are interesting also in photovoltaics,[5] in diluted magnetic semiconductors,[6] and have already found practical applications as tunable filters and ultraviolet photodetectors.[7,8]

High-pressure (HP) studies on $A^{II}B_2^{III}X_4^{VI}$ compounds are receiving increasing attention in the last years.[9–26] In particular, the AGa_2Se_4 (A = Mn, Zn, and Cd) family has been studied by X-ray diffraction (XRD), Raman spectroscopy, and optical absorption. However, only few works have been devoted to the study of $HgGa_2Se_4$ under pressure. Recently, we reported optical absorption studies of DC-$CdGa_2Se_4$ and DC-$HgGa_2Se_4$ under pressure and focused on the explanation of the strong non-linear pressure dependence of their

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