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Optical absorption of defect chalcopyrite and defect stannite $ZnGa_2Se_4$ under high pressure

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ABSTRACT

Optical absorption measurements at high pressure have been performed in two phases of the ordered-vacancy compound (OVC) $ZnGa_2Se_4$: defect stannite (DS) and defect chalcopyrite (DC). The direct bandgap energy of both phases exhibits a non-linear pressure dependence with a blueshift up to 10 GPa and a redshift at higher pressures. We discuss the different behavior of both phases in these two pressure ranges in relation to the pressure-induced order-disorder processes taking place at cation sites. Measurements performed in both phases on downstroke after increasing pressure to 22 GPa show that the direct bandgap energy of the recovered samples at room pressure was 0.35 eV smaller than that of the original samples. These results evidence that different disordered phases are formed on decreasing pressure, depending on the cation disorder already present in the original samples. In particular, we attribute the recovered samples from the original DC and DS phases to disordered CuAu (DCA) and disordered zincblende (DZ) phases, respectively. The decrease of the direct bandgap energy and its pressure coefficient on increasing disorder in the four measured phases are explained. In summary, this combined experimental and theoretical work on two phases (DC and DS) of the same compound has allowed us to show that the optical properties of both phases show a similar behavior under compression because irreversible pressure-induced order-disorder processes occur in all adamantine OVCs irrespective of the initial crystalline structure.

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