Lattice dynamics study of $HgGa_2Se_4$ at high pressures

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Abstract

We report on Raman scattering measurements in mercury digallium selenide ($HgGa_2Se_4$) up to 25 GPa. We also performed, for the low-pressure defect-chalcopyrite structure, lattice-dynamics *ab initio* calculations at high pressures which agree with experiments. Measurements evidence that the semiconductor $HgGa_2Se_4$ exhibits a pressure-induced phase transition above 19 GPa to a previously undetected structure. This transition is followed by a transformation to a Raman-inactive phase above 23.4 GPa. On downstroke from 25 GPa till 2.5 GPa a broad Raman spectrum was observed, which has been attributed to a fourth phase, and whose pressure dependence was followed during a second upstroke. Candidate structures for the three phases detected under compression are proposed. Finally, we also report and discuss the decomposition of the sample by laser heating at pressures close to 19 GPa. As possible products of decomposition we have identified at least the formation of trigonal selenium nanoclusters and cinnabar-type HgSe.

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