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Mechanical properties and Raman scattering investigation under indentation of $CdGa_2S_4$ and $CdGa_2Se_4$

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Abstract

The behavior of $CdGa_2S_4$ and $CdGa_2Se_4$ single crystalline semiconductors under Berkovich indentation of the (1 1 2) face in the load range of 10–700 mN has been investigated. Values of hardness and Young's modulus have been determined for this load range. A comparative analysis of crack development under indentation was performed for these two compounds. The observed indentation size effect was analyzed from the point of view of energy consumed for the formation of the residual imprint, fracture and relaxation processes. It was found that crack development affects the energy-load and hardness-load dependences, which show specific features for each compound. The effect of indentation on eventual phase transitions was investigated by comparing the micro-Raman spectra from a non-indented site with those measured in the indentation. Evidence of a phase transition under indentation from the initial defect chalcopyrite structure to a disordered zincblende phase is found.

Keywords: indentation, hardness, deformation energy, fracture, phase transition, Raman spectroscopy

(Some figures may appear in colour only in the online journal)

1. Introduction

$CdGa_2S_4$ and $CdGa_2Se_4$ semiconductor compounds belong to a class of so-called $A^{II}B_2^{III}X_4^{VI}$ ordered-vacancy compounds (OVCs) characterized by the lack of cubic symmetry and by an unbalanced number of cations (A and B) and anions (X) which results in the occupation of a cation site by a vacancy in an ordered and stoichiometric fashion. These compounds demonstrate rather strong anisotropy, nonlinear optical properties and birefringence which make them suitable for many technological [1–4] and optoelectronic applications, such as solar cells, nonlinear optical devices, narrow-band optical filters, tunable filters and ultraviolet photodetectors [5–8].

High-pressure (HP) studies on these compounds have received increasing attention in recent years because these studies can help to understand the relationship between the properties and structures of materials which could have profound implications in many fields. Particularly, comprehensive works on pressure induced effects, phase transitions and order–disorder processes under hydrostatic pressure, created in diamond anvil cells for $CdGa_2S_4$ [9, 10] and $CdGa_2Se_4$ [9, 11, 12] have been published. Pressure induced effects are closely related to elastic constants, elastic moduli and other mechanical properties of materials. Calculated data of these properties, particularly the bulk, shear and Young moduli of $CdGa_2S_4$ and $CdGa_2Se_4$ have been reported in comparison to $HgGa_2S_4$ and $HgGa_2Se_4$ in several recent works [13–15]. On the other hand, scarce data are available on the hardness of these materials. Particularly, Chess *et al* [16] reported the hardness of hot-pressed ceramic discs of

