Comparative Study of SnS$_x$Se$_{2-x}$ alloys by High Pressure Raman Spectroscopy

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In this work, the hydrostatic pressure response of the phonon modes of ternary SnS$_x$Se$_{2-x}$ ($x=0.6, 0.8, 1$) alloys has been studied by means of Raman spectroscopy. High pressure (up to 8 GPa) was generated using a gas membrane-type diamond anvil cell. Owing to the two-mode behaviour of the E$_g$ and A$_{1g}$ modes in the ternary dichalcogenide alloys investigated [1], four Raman bands are observed at ambient conditions and the frequency evolution of three of them {E$_g$(SnSe$_2$-like), A$_{1g}$(SnSe$_2$-like) and A$_{1g}$(SnS$_2$-like)} was followed with pressure. Upon pressure application, all Raman peaks monotonically shift to higher frequencies due to the volume reduction and the bond strengthening (Figure 1).

![Raman peaks](image)

**Figure 1:** Pressure evolution of the frequencies of the clearly resolved Raman peaks in the SnS$_x$Se$_{2-x}$ alloys. Open (closed) circles correspond to pressure increase (decrease).

The pressure coefficient of the A$_{1g}$(SnS$_2$-like) peak frequency increases gradually from 3.60 to 3.93 cm$^4$/GPa$^{-1}$ with increasing S content, $x$. These values are compatible with those reported in the literature for the binary SnS$_2$ [2]. At the same time, the pressure coefficient of the A$_{1g}$(SnSe$_2$-like) peak frequency decreases from 3.08 to 2.72 cm$^4$/GPa$^{-1}$ with $x$, being always larger than that observed for the binary SnSe$_2$ [2]. Furthermore, contrary to the strong covalent bonding along the $a$-axis compared to the weak van der Waals interactions along the $c$-axis, the in-plane E$_g$(SnSe$_2$-like) mode exhibits larger pressure coefficient than those of the A$_{1g}$ modes along the $c$-axis in all the studied alloys. We also extracted the Grüneisen parameters for the A$_{1g}$(SnSe$_2$-like): 0.35, 0.34, 0.36 and the A$_{1g}$(SnSe$_2$-like) mode: 0.44, 0.41, 0.37 for $x=0.6, 0.8$ and 1, respectively. These values indicate the stronger Sn-S interaction along the $c$-axis compared to the Sn-Se one in the ternary alloys, in agreement with the existing X-ray diffraction (XRD) data in the literature [3].

References


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