

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

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In this work, the hydrostatic pressure response of the phonon modes of ternary  $\text{SnS}_x\text{Se}_{2-x}$  ( $x=0.6, 0.8, 1$ ) 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  $\{E_g(\text{SnSe}_2\text{-like}), A_{1g}(\text{SnSe}_2\text{-like})$  and  $A_{1g}(\text{SnS}_2\text{-like})\}$  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).

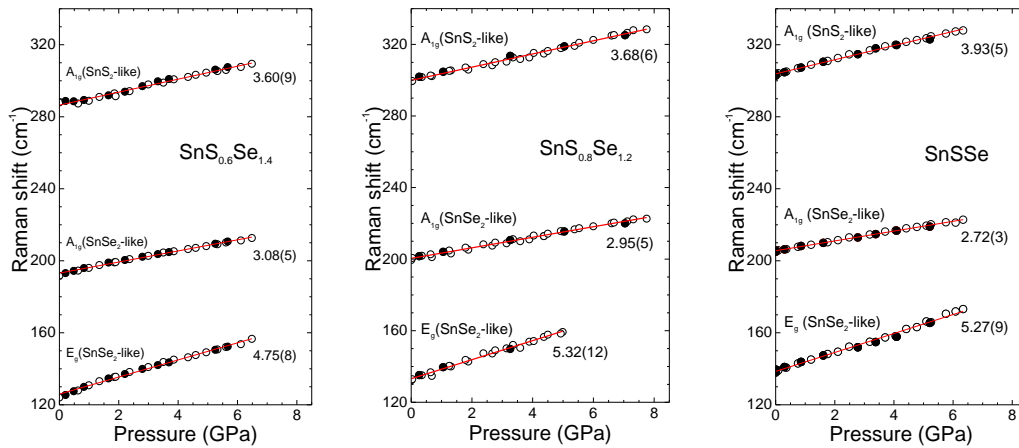


Figure 1: Pressure evolution of the frequencies of the clearly resolved Raman peaks in the  $\text{SnS}_x\text{Se}_{2-x}$  alloys. Open (closed) circles correspond to pressure increase (decrease).

The pressure coefficient of the  $A_{1g}(\text{SnS}_2\text{-like})$  peak frequency increases gradually from 3.60 to 3.93  $\text{cm}^{-1}\text{GPa}^{-1}$  with increasing S content,  $x$ . These values are compatible with those reported in the literature for the binary  $\text{SnS}_2$  [2]. At the same time, the pressure coefficient of the  $A_{1g}(\text{SnSe}_2\text{-like})$  peak frequency decreases from 3.08 to 2.72  $\text{cm}^{-1}\text{GPa}^{-1}$  with  $x$ , being always larger than that observed for the binary  $\text{SnSe}_2$  [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  $E_g(\text{SnSe}_2\text{-like})$  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  $A_{1g}(\text{SnS}_2\text{-like})$ : 0.35, 0.34, 0.36 and the  $A_{1g}(\text{SnSe}_2\text{-like})$  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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