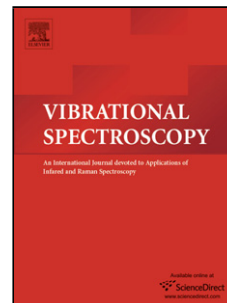


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Low-Temperature Raman Studies of Sulfur-Rich $\text{TlIn}(\text{S}_{1-x}\text{Se}_x)_2$ Single Crystals

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Graphical abstract



Abstract

Raman spectra of $\text{TlIn}(\text{S}_{1-x}\text{Se}_x)_2$ ($0 \leq x \leq 0.25$) single crystals in the frequency range 16–400 cm^{-1} were studied at $T = 30$ K in the $Z(\text{XX}+\text{XY})\bar{Z}$ configuration. The experimental Raman spectra of $\text{TlIn}(\text{S}_x\text{Se}_{1-x})_2$ single crystals were analyzed by multi-peak simulation by Lorentzian contours, enabling the peak frequencies, halfwidths and intensities to be determined. Their compositional dependences were studied. Compositional behaviour of Raman features revealed in the spectral regions 40–85 cm^{-1} and 190–220 cm^{-1} is discussed in view of different number of isovalent S and Se atoms in structural groups corresponding to the general formula of $\text{In}_4\text{S}_{10-y}\text{Se}_y$.

Keywords: Raman scattering; layered crystals; crystal disorder

1 Introduction

Solid solutions of chalcogenide-based ferroelectric single crystals attract a considerable scientific interest due to the existence of incommensurate modulated structures as well as polycritical points in the pressure–temperature (p, T) and composition–temperature (x, T) dependences [1,2]. Interesting objects for such studies are TlMX_2 -type crystals ($\text{M} = \text{Ga, In, X} = \text{Se, S}$) characterized by layered or chain-like structure. They were the first low-dimensional semiconductors, for which a series of phase transitions with modulated structures was discovered [3,4]. A special case is TlInS_2 , for which, based on experimental and theoretical studies, a sequence of phase transitions (PTs) as well as an incommensurate phase in the range of 190–220 K [3,4] and a complex (p, T) phase diagram are reported [5–9].

Note that the temperature behaviour of the dielectric constant in $\text{TlIn}(\text{S}_{1-x}\text{Se}_x)_2$ mixed crystals in the temperature interval including the phase transition range (190–216 K)

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