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Understanding the effects of dopant impurities on quaternary chalcogenide system properties by investigating and modeling local vibrational modes and Raman lineshapes PRASHANT SARSWAT, MICHAEL FREE, University of Utah — $Cu_2ZnSnS_xSe_{4-x}$ (CZTSSe) has gained attention as a p-type absorber layer due to its attractive properties such as optimum band gap, high absorption coefficient, and use of low cost elements. However, impurities in CZTSSe produce detrimental effects, which limit the device performance. Phonon dispersion in most of the semiconductors is found to be susceptible to the pairing between atoms within the lattice. Hence, a change in phonon dispersion can be used to investigate the effects of foreign impurities on such pairing. Thus a series of experiments were conducted to investigate the effect of free holes on the optical phonons of doped CZTSSe system as well as to evaluate asymmetry in the Raman lineshape. When irradiated with photons, doped CZTS possibly produces a continuum of inter-valence band electronic excitations, which can envelop the Raman-active phonon energy. Such overlap between the electronic continuum and discrete state can cause interference effects in CZTSSe. It was observed that Raman lineshape becomes more asymmetric, wider, and shifts towards lower frequency when laser power density increased. All these observations were found for Raman A mode as well as E (TO, LO) mode for doped CZTSSe samples.

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