# Raman characterization and modeling of $Cu_2ZnSn_{1-X}Ge_XS_4$ single crystals grown using chemical vapor transport

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**Abstract:** Reported in this paper are the results of investigations aimed at $Cu_2ZnSn_{1-X}Ge_XS_4$ single crystals. A detailed study of Raman spectra at room temperature and 80 K for crystals synthesized in two one-type

processes was performed. It has been shown that even insignificant temperature fluctuations during the synthesis can cause changes of elemental composition in these compounds. The analysis of the Raman spectra inherent to the grown samples confirms that they crystallize in the kesterite structure. It has been ascertained that, when the Ge content increases, the Raman spectra of $Cu_2ZnSn_{1-X}Ge_XS_4$ show a two-mode reconstruction of both full-symmetric bands related with sulfur atom vibration in $Sn-S_4$ and $Ge-S_4$ tetrahedra. These experimental bands have been described by theoretical curves calculated within the framework of a bound oscillator model. Based on this model, one can adequately describe the changes both in the band intensity and frequency position for various elemental compositions.

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