

Strength of electron-phonon scattering induced by Bi-doping in thermoelectric $\text{Ge}_{0.92-y}\text{Sb}_{0.08}\text{Bi}_y\text{Te}$ ($y=0.04$ and 0.06) single crystals (proposal 24802)

Wen-Hsien Li¹, Yu-Shan Tseng¹, Huei-Yin Tseng¹, Hung-Cheng Wu², Tung-Yuan Yung³

¹Department of Physics, Soochow University, Taipei, Taiwan

²Department of Physics, National Sun Yat-Sen University, Kaohsiung, Taiwan

³Department of Material Research, National Atomic Research Institute, Taiwan

The solar energy conversion efficiencies of methylammonium (CH_3NH_3 , MA) lead iodide ($\text{CH}_3\text{NH}_3\text{PbI}_3$) perovskite solar cells have demonstrated to increase tremendously from 3.8% to over 22.1%. ($\text{CH}_3\text{NH}_3\text{PbI}_3$) is also found to have unusual properties, such as acoustic-optical phonon up-conversion caused hot-phonon bottleneck effect and unexpected ultra-low thermal conductivity of ~ 0.5 W/mK at 300 K, which is even lower than that of amorphous silicon. In this proposal we aim to complete the investigation made on the effects of coupling between the $(\text{CH}_3\text{NH}_3)^+$ cations and the PbI_3^- framework on the lattice periodicity and $(\text{CH}_3\text{NH}_3)^+$ vibrations. Six dispersion-less excitations, that were identified to be the vibration modes of the CH_3NH_3^+ cations, were detected at low temperatures (Figs. 1a and 1b) in our INS experiments performed on GPTAS in June 2024. Thermal variations of the energy and intensity (Fig. 2) of the vibration modes reveal an anomaly at 120 K. An additional excitation at ~ 8 meV (marked V7 in Fig. 1c) appears at the excitation spectra taken at 128 K (Fig. 1c) and 166 K (Fig. 1d) and 175 K (Fig. 1e), but disappeared at 213 K (Fig. 1f). In addition, the excitation spectrum taken at 166 K (Fig. 1d) and at 175 K (Fig. 1e) are very different, reflecting a significant change in structure of the $(\text{CH}_3\text{NH}_3)^+$ sublattice between 166 and 175 K. Excitation spectra in finer temperature steps are needed to uncover this lattice change. ICM reflections from this crystal were indeed observed during the crystal alignment. This is the only Bragg reflection data we obtained in last experiments on GPTAS. More diffraction data that reveal lattice incommensurability, and thermal evolution of the ICM phase are needed to link the changes in vibration modes of the CH_3NH_3^+ cations to the lattice incommensurability.

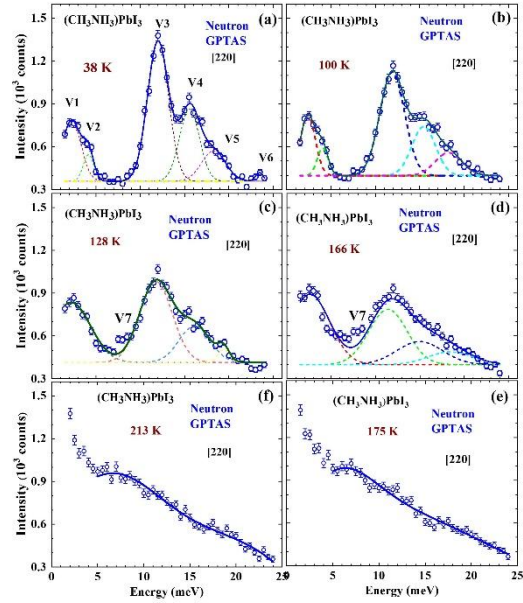


Figure 1. The excitation patterns detected at six representative temperatures; Six excitations were observed at 38 K, but all six excitations disappeared above 213 K and development of an excitation, marked V7, above 128 K.

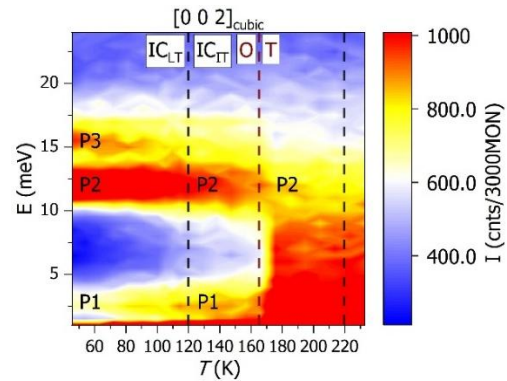


Figure 2. Variations of excitation intensity covering 40 to 240 K. Excitation intensities renormalized into background intensity above 170 K.