

Unveiling tetrahedral dynamics in 0-D halide perovskite $\text{Cs}_3\text{Cu}_2\text{I}_5$

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To determine the acoustic phonon dispersion and phonon velocity of $\text{Cs}_3\text{Cu}_2\text{I}_5$, inelastic neutron scattering measurements were performed using the HODACA cold neutron triple-axis spectrometer. A 1.5 g $\text{Cs}_3\text{Cu}_2\text{I}_5$ single crystal was used in this experiment, as shown in Fig. 1. The crystal was aligned in the $[020]$ – $[101]$ scattering plane to investigate its low-energy phonon excitations. Measurements were carried out at 200, 300, and 400 K. The energy scans covered the range from 0 to 3 meV with a step size of 0.2 meV. To ensure sufficient counting statistics at each temperature, the measurement conditions were set to $\text{mcu} = 5$ at 200 K, $\text{mcu} = 6$ at 300 K, and $\text{mcu} = 7$ at 400 K. The measured inelastic neutron scattering spectra along the $[2K2]$ direction at different temperatures are presented in Fig. 2, providing the basis for determining the acoustic phonon energies and extracting the corresponding phonon velocities.

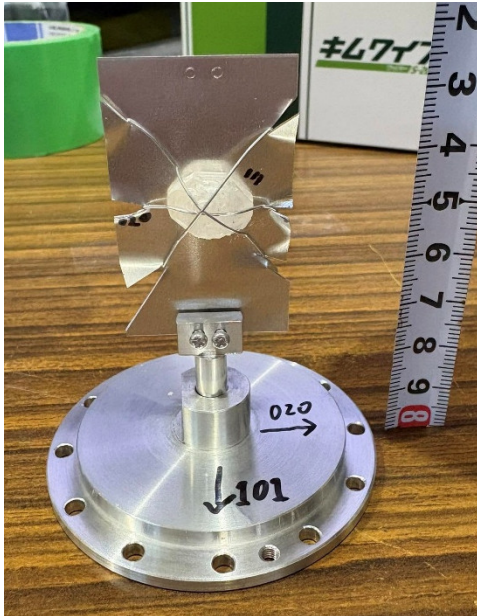


Fig. 1. Photograph of the $\text{Cs}_3\text{Cu}_2\text{I}_5$ single crystal used for the INS measurements. The crystal was aligned in the $[020]$ – $[101]$ scattering plane.

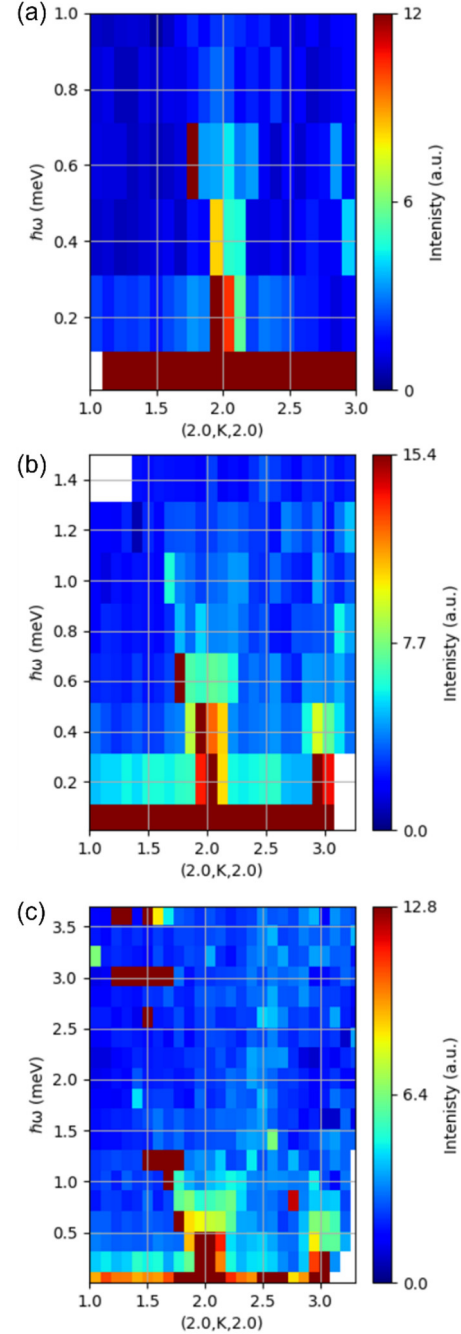


Fig. 2. Phonon dispersion relations of $\text{Cs}_3\text{Cu}_2\text{I}_5$ measured along $(2K2)$ measured at (a) 200 K, (b) 300 K, and (c) 400 K.