Unveiling the phonon instability in SnSe single crystals before superionic phase transition

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This experiment was conducted as a direct follow-up to our previous inelastic neutron scattering (INS) study performed at HODACA in June 2024. In the previous study, pronounced phonon softening was observed in the Pnma phase of SnSe upon heating from 300 K to 700 K. To improve the statistical quality of the measurements, more rigorous experimental conditions were adopted in the present experiment. Specifically, the energy scan step was refined to a high-resolution interval of 0.2 meV, and the counting time at each measurement point was increased to 2 mcu. The present experiment focused on measuring the phonon dispersion relations below 6 meV at 700 K, and the resulting data are shown in Fig. 1(a–d). Owing to the significantly improved counting statistics, the acoustic and optical phonon dispersion curves are much more clearly resolved than those obtained previously.

To better visualize the phonon dispersion of SnSe along different crystallographic directions, we employed the *Asyura* software developed by Dr. Hodaka to reconstruct the three-dimensional (3D) phonon dispersion from the experimental data, as shown in Fig. 1(e–f). C Compared with conventional two-dimensional representations, the 3D visualization provides a more comprehensive view of the phonon dispersion throughout reciprocal space and enables a more intuitive examination of the anisotropic phonon dispersion along different crystallographic directions. In addition, the reconstructed 3D phonon dispersion clearly reveals the phonon softening and enhanced phonon scattering associated with the *P*nma–*C*mcm phase transition in SnSe. These results provide valuable experimental information for understanding the evolution of lattice dynamics during the phase transition and serve as an important basis for further investigating the microscopic origin of the pronounced thermal conductivity anisotropy in SnSe.

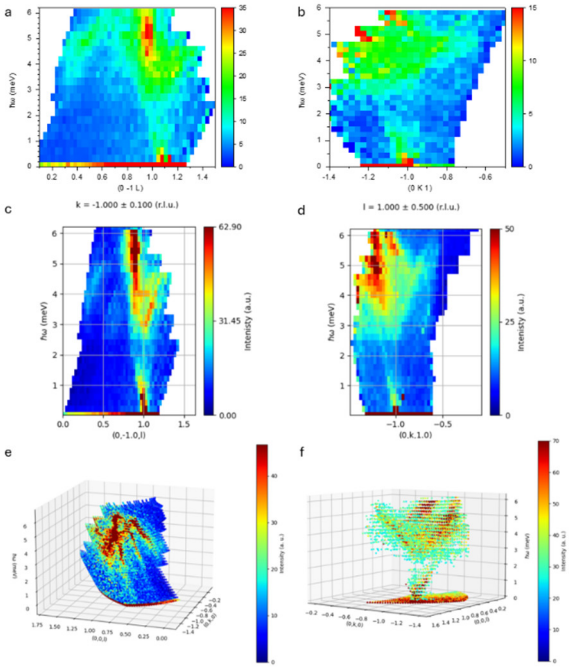

Fig. 1 (a-d) Phonon dispersion relations of SnSe measured at 700 K using the HODACA triple-axis spectrometer. (e,f) 3D visualization of the phonon dispersion relations of SnSe reconstructed from the experimental data.