Thickness dependence of the Raman spectrum of antiferromagnetic $NiPS_3$

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Abstract

Lattice vibrations in few-layer $NiPS_3$ were studied by Raman spectroscopy with five different excitation sources. In the low-frequency Raman spectra, shear and breathing modes arising from rigid vibrations of entire layers were observed, providing insights into interlayer interactions. These interactions were quantified using linear chain model calculations down to bilayer $NiPS_3$. Additionally, the low-frequency Raman spectra serve as a unique, reliable tool for determining the number of layers. The most striking feature in the high-frequency range (>100 cm^{-1}) is the Davydov splitting of an A_{1g} mode at ~ 255 cm^{-1} at 4 K. The weak interlayer interaction splits the mode into multiple peaks, depending on the number of layers, offering an alternative method for layer number determination.

Figures

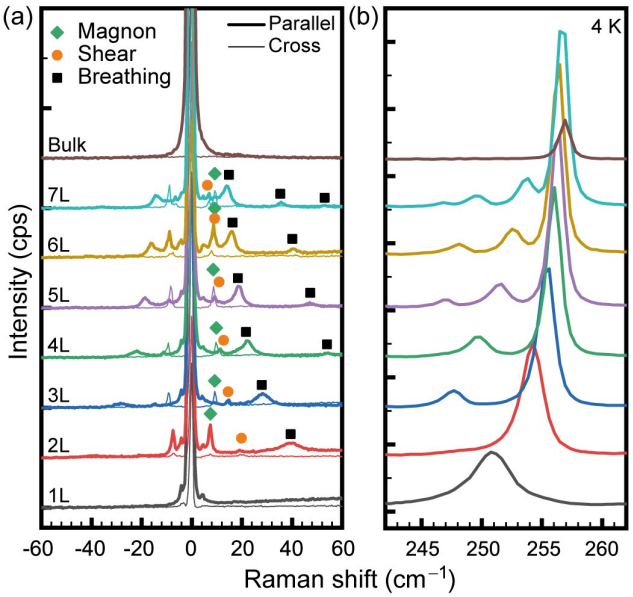

Figure 1: Raman spectra of 1-7 L and bulk $NiPS_3$ samples at 4 K (a) in the low-frequency region and (b) the Davydov splitting in the high-frequency regions.