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Phonon renormalization in LaCoO_3

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LaCoO_3 features two broad crossovers observed around $T_1 = 100$ K and $T_2 = 200$ K. These crossovers are typically associated with the temperature dependent population of excited spin states of the Co^{3+} ion, which evolves upon heating from the low-spin (LS), $S = 0$, to high-spin (HS), $S = 2$, configuration. Since the CoO_6 octahedra expands around the larger HS sites, a static LS-HS order was proposed by Goodenough in the 1960's [1] but was never confirmed experimentally. More recent studies [2,3] propose a dynamic short-range order of alternating LS and HS Co sites. A corresponding dynamic distortion of the crystal lattice mimics closely the Co-O breathing mode. Here, we use inelastic neutron scattering to study the lattice dynamics of LaCoO_3 over a wide temperature range, $5 \text{ K} \leq T \leq 700 \text{ K}$. We find strong phonon renormalization of low- as well as high-energy phonon modes with periodicities corresponding to the proposed superlattice.

[1] P. M. Raccah and J. B. Goodenough, Physical Review 155, 932 (1967).

[2] J. Kuneš and V. Křápek, Physical Review Letters 106, 256401 (2011).

[3] V. Křápek et al., Physical Review B 86, 195104 (2012).

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