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Lattice Dynamics of (ND4Br)x(KBr)1-x Mixed Crystals

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Abstract : We have incorporated the translational rotational (TR) coupling effects in the framework of three body force shell model (TSM) to develop an extended TSM (ETSM). The dynamical matrix of ETSM has been applied to compute the phonon frequencies of orientationally disordered mixed crystal (ND4Br)x(KBr)1-x in (q00), (qq0) and (qqq) symmetry directions for compositions $0.10\≤x\≤0.50$ at T=300K. These frequencies are plotted as a function of wave vector k. An unusual acoustic mode softening is found along symmetry directions (q00) and (qq0) as a result of translation-rotation coupling.

Keywords: orientational glass, phonons, TR-coupling, lattice dynamics

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