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Lattice dynamics of Pb(Mn1-xFex)BO4 (x = 0, 0.5 1.0) studied by inelastic neutron scattering

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The mullite-type PbMnBO4 and PbFeBO4 phases have been considered as excellent playground to follow the Goodenough–Kanamori–Anderson spin rules to understand the antiferromagnetic (AFM) and ferromagnetic (FM) microscopic features. We report inelastic neutron scatterings (INS) of PbFeBO4, PbMnBO4 and Pb(Fe0.5Mn0.5)BO4 powder samples between 1.5 K and 520 K. The Stokes and anti-Stokes spectra are collected on IN4C@ILL and IN6@ILL, respectively. The temperature-dependent dynamic structure factor S(Q,E) demonstrates clear changes of phonon dynamics across the magnetic phase transitions at the respective TC. The INS profile of PbFeBO4 exhibits steep magnon excitations up to E ⊠ 15 meV at the momentum transfer of Q = 1.1(1), 1.6(1) and 2.7(1) Å-1, which are corresponding to acoustic spin-waves centered at (010), (111) and (113) AFM Bragg reflections, respectively. An AFM spin-wave velocity at d = 0.57(1) nm is estimated to be 653(24) ms-1. The analysis of the temperature-dependent low-frequency phonon profile is challenging below and above the TC due to magnon-phonon coupling and strong paramagnetic background, respectively. However, phonon density of states (PDOS) of the isostructural non-magnetic PbAlBO4 and PbGaBO4 phases help understand the associated phonons across the respective TC. Ab-initio lattice dynamical calculations of PDOS enables microscopic interpretations of the observed data. The calculations well reproduce the observed vibrational features and provide the partial vibrational components. Temperature-dependent PDOSs demonstrate that the optically silent phonon features exhibit negative mode Grüneisen parameter, which are responsible for the axial negative thermal expansion for all relevant mullite-type compounds.

Hauptautoren: Prof. MURSHED, M. Mangir (University of Bremen); Herr GOGOLIN, Mathias (University of Bremen); Dr. KOZA, Michael Marek (Institut Laue Langevin); Dr. CHOGONDAHALLI MUNIRAJU, Naveen Kumar (Institute of Nuclear Physics PAN); Prof. GESING, Thorsten M. (University of Bremen)

Sitzung Einordnung: Mounting Posters, Beer and light Dinner

Track Klassifizierung: Magnetism & Superconductivity