



## Lattice dynamics of $\text{Pb}(\text{Mn}_{1-x}\text{Fe}_x)\text{BO}_4$ ( $x = 0, 0.5, 1.0$ ) studied by inelastic neutron scattering

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The mullite-type  $\text{PbMnBO}_4$  and  $\text{PbFeBO}_4$  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  $\text{PbFeBO}_4$ ,  $\text{PbMnBO}_4$  and  $\text{Pb}(\text{Fe}_{0.5}\text{Mn}_{0.5})\text{BO}_4$  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  $\text{PbFeBO}_4$  exhibits steep magnon excitations up to  $E \approx 15$  meV at the momentum transfer of  $Q = 1.1(1)$ ,  $1.6(1)$  and  $2.7(1)$   $\text{\AA}^{-1}$ , 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<sup>-1</sup>. 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  $\text{PbAlBO}_4$  and  $\text{PbGaBO}_4$  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.

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**Sitzung Einordnung:** Mounting Posters, Beer and light Dinner

**Track Klassifizierung:** Magnetism & Superconductivity