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Multiferroic Pb(Fe$_{1/2}$Nb$_{1/2}$)O$_3$ Single Crystals: A Raman scattering study

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Among complex perovskite-type structure multiferroics [A(B´B´´)O$_3$], lead iron niobate Pb(Fe$_{1/2}$Nb$_{1/2}$)O$_3$ (PFN) discovered by Smolenskii et al. 1 is currently of interest because of its high dielectric constant diffuse phase transition and magnetoelectric effect. PFN presents ferroelectric transition below $T_C$ ~ 350-395 K and antiferromagnetic transition below $T_N$ ~ 145 K.

In PFN, the Pb$^{2+}$ cations with a lone electron pair in A site and the relative displacements of oxygen and Fe$^{3+}$/Nb$^{5+}$ ions in the octahedral B sites favor the electric ordering whereas the Fe$^{3+}$ cations with partially filled d orbitals contribute to the magnetic ordering. Because of its complex structure, still exists a disagreement about the crystalline structure of PFN: monoclinic (space group Cm), rhombohedral (space group R3m), and cubic (space group Pm3m) structure symmetry at room temperature were reported.

In this work, we report temperature-dependent Raman spectra (10-500 K) in the frequency range of 150-1250 cm$^{-1}$ of cubic PFN single crystals, complemented with magnetization measurements. We want to provide microscopic information in this material.

Over the range from 150 to 950 cm$^{-1}$, very broad and overlapping peaks (first-order character) were observed in the overall studied temperature range possibly due to local distortions which are characteristic in this kind of Pb-based complex perovskite. Also, a prominent high-frequency peak at ~1130 cm$^{-1}$, which we assign as a two-phonon peak, was observed (see Fig. 1).

Temperature dependence of the Raman spectra showed an anomaly in a characteristic temperature $T^* ~ 330$ K. Here, drastic changes in the Raman scattering intensity and spectral shape were observed with temperature variations, such as the appearance of new first- and second-order peaks below $T^*$. The temperature behavior of the two-phonon peak shows a strong electron-phonon interaction in PFN. Also, since it was reported weak magnetic ordering at and even above room temperature in
this material, the anomaly at $T^* \sim 330$ K by Raman scattering could be possibly suggesting an interplay between magnetic and ferroelectric orders.

\begin{figure}[h]
\centering
\includegraphics[width=0.6\textwidth]{raman_spectra.png}
\caption{Raman spectra as a function of temperature in Pb(Fe$_{12}$Nb$_{12}$)O$_3$.}
\end{figure}

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**REFERENCES**