[MS34-P06] Polar nanoregions and diffuse scattering in relaxor ferroelectrics.
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We present a fully atomistic model of polar nanoregions (PNRs) in the relaxor ferroelectric $PbMg_{1/3}Nb_{2/3}O_3$. Our molecular dynamics calculations [1] reproduce both the characteristic form of the neutron diffuse scattering distribution and its temperature dependence. A shell model was used with a modified version of a published interatomic potential that was based on ab initio calculations. The parameters of this potential were optimized for the present work to provide a better description of the O atom interactions, as these are particularly important for neutron scattering. At high temperatures the Pb ions are displaced from their mean site positions in a direction that has an isotropic distribution, but at low temperatures the distribution condenses into eight localized sites displaced from the average position along each of the eight possible □111□ directions. At intermediate temperatures (300 K) the distribution is cuboidal with some preference for□111□ displacements but with all possible displacement directions present. Longitudinal correlations between the displacements of Pb-Mg/Nb and Pb-O increase monotonically in magnitude as the temperature changes from 700 K to 10 K with the sign of the Pb-O correlation being negative. At low temperatures this increase in correlation results in polar nanoregions that are clearly visible in plots of the local structure, although the exact form of these domains is more difficult to visualize. We show that the form of these PNRs can be revealed by an examination of conditional displacement distributions at low temperatures. Therein strongly anisotropic cooperative displacement behaviour is found. Remnants of this correlation pattern persist at much higher temperatures, but progressively a relatively smaller proportion of the Pb ions appears to be taking part and there is a substantially larger random component. It seems likely that the onset of the characteristic structured diffuse scattering at around 400 K coincides with the appearance of this cooperative displacement behaviour.

[1] M. Pasciak, T. R. Welberry, J. Kulda, M. Kempa and J. Hlinka Phys. Rev. B 85, 224109 (2012).

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