A study of the disorder in heavily doped Ba$_{1-x}$La$_x$F$_{2+x}$ by neutron scattering, ionic conductivity and specific heat measurements

The ionic disorder in single crystals of the fluorite-type solid solutions Ba$_{1-x}$La$_x$F$_{2+x}$ (with $x=0.209$ and $x=0.492$) has been studied in the temperature range from room temperature to 800 degrees C by diffuse neutron scattering, ionic conductivity, and specific heat measurements. From the diffuse neutron scattering it was found that the disorder was dominated by 222 clusters, which at low temperatures ($T>10^{-10}s$), in agreement with NMB results which suggest a jump frequency below 75 MHz. The temperatures at which the steepest slopes are found in the loss of correlations and in the conductivity coincide at approximately 650 degrees C. At this temperature no clear anomaly is observed in the specific heat. Based on these findings the authors propose a conduction mechanisms where F- ions are moving through the lattice by means of rearrangements of the 222 clusters.

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