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Distortions and Superstructure in Inverse Perovskite Nitrides

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We discovered nitrogen/defect ordering leading to elpasolite-type superstructures in inverse perovskites with the general composition $(A_3N_x)Tt$ ($A = Ca, Sr, Ba$; $Tt = Si, Ge, Sn, Pb$). Due to the large scattering length of nitrogen, neutron powder diffraction is crucial when it comes to illuminating the nature of these superstructures.

For example, high quality powder X-ray diffraction patterns of nitrogen-deficient $(Ca_3N_x)Sn$ and $(Ca_3N_x)Pb$ feature barely visible reflections indicating an elpasolite-type ordering, but yield next to no information as to the extent of this ordering. The problem is compounded when looking at $(Ba_3N_x)Sn$ and $(Ba_3N_x)Pb$, where the slight shift of barium atoms toward occupied nitrogen sites contributes much more strongly to the superstructure reflections in X-ray patterns than the occupation of the nitrogen sites itself. By contrast, the same reflections are among the strongest peaks in neutron diffraction patterns of these compounds and it is mostly the nitrogen ordering itself eliciting them.

In addition to the superstructure, $(Ba_3N_x)Sn$ and $(Ba_3N_x)Pb$, as well as the hitherto unknown compounds $(Ca_3N_x)Si$, $(Sr_3N_x)Ge$ and $(Ba_3N_x)Ge$, feature distortions of the perovskite structure due to octahedral tilting. This makes the crystals undergo multiple twinning processes upon cooling down from the temperature of synthesis, which renders analysis by single crystal diffraction exceedingly difficult.

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