Honeycomb Diffuse Intensities in NaREF₄ Upconversion Materials

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Hexagonal sodium rare-earth (RE) fluorides, e.g. NaYF4: Yb, Er, are very efficient upconversion materials which emit visible light upon infrared excitation. The efficiency of the upconversion process depends mainly on the doping ratio, the phase purity and the Na:RE ratio. These phases have hexagonal structures with a disordered cation distribution. Here we report a detailed investigation of Na_{1.5}La_{1.5}F₆. The reconstructed layers of reciprocal space contain either sharp Bragg reflections for integer values of l, or planes with honeycomb like diffuse intensities for half-integer values of l (Fig left: h k 1.5). The Bragg reflections indicate a hexagonal metric and the average structure could be refined with space group symmetry P-6. It shows three different columns of cations with Na, La or a 1:1 ratio of both (Fig right). The diffuse intensities are well reproduced if it is assumed that Na and La alternate regularly in the disordered columns along c and that Na and La alternate with a probability less than one in the **a**,**b** plane



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