

NANO-SCALE INHOMOGENEITY IN NiO

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The aim of this work was to study the inhomogeneity of NiO (and Ni_{1-x}Li_xO) single crystals grown by floating zone melting. Different types of inhomogeneities varied from mm-scale to nano-scale were observed by X-ray diffraction, electron microscopy, LEED, AFM and STM/STS. In particular, AFM/STM images reveal the unusual granular structures onto NiO(100) surface with a typical granula size of a few nanometers. The nano-granular structure was also studied by low-energy electron diffraction (LEED) and transmission electron microscopy (TEM). The estimation of coherent area size from width of LEED spots and TEM images is in good agreement with STM - AFM data. The first principles calculations shown that the possible reason of the nanogranular structure formation is the lattice distortions induced by Ni vacancy. According to the DFT calculations the diameter of the area of the atomic displacements around the Ni vacancy is 1.2 nm. That is very close to the size of the granules observed by STM.