Rumpled Surface Structure and Lattice Dynamics of NiO(001)

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Abstract

Rumpled surface structure and root mean square (rms) thermal vibration amplitudes of NiO(001) were determined by high-resolution medium energy ion scattering. The clean 1×1 surface was prepared by cleavage in the air and annealing at 500°C for 40 min in O_2-pressure of 1×10^{-4} Torr. The interlayer distance between the top- and 2nd-layer is contracted by 1.44±0.7 % and the top-layer Ni-plane is displaced by 0.10±0.01Å toward the vacuum side relative to the top-layer O-plane. The present result is consistent with the recent *ab initio* calculation based on the density functional theory using the local spin density approximation. We also determined the rms thermal vibration amplitudes of Ni and O atoms in the bulk and in the top-layer. The result obtained is compared with that calculated using the pair potential proposed by Lewis and Catlow.

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