Surface Structure of Y_2O_3(9.5 mol%)-stabilized ZrO_2(001) Determined by High-resolution Medium Energy Ion Scattering

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Abstract

The surface structure of single crystalline ZrO_2(001) stabilized with Y_2O_3(9.5 mol%) (YSZ) was determined by high-resolution medium energy ion scattering (MEIS). The clean 1×1 surface was prepared by a chemical treatment followed by annealing at 600 °C in O_2 atmosphere (1×10^{-5} Torr). The ion channeling combined with the blocking effect using 80 keV He^+ ions showed that the surface is strongly reconstructed and takes the form of a rumpled Zr(Y)O plane, where the O atoms are located on the center of the square of the Zr(Y) sublattice. The positions of the top layer O and Zr(Y) atoms measured from the underlying Zr(Y) plane are displaced toward the vacuum side by 0.11±0.04 Å and 0.045±0.02 Å, respectively compared with the bulk interplanar distance. Analysis by the impact collision ion scattering spectroscopy using 1.8 keV He^+ ions supported the above surface structure and suggested that about 10 % of the top layer O sites are vacant. The present MEIS analysis also revealed the fact that the thermal vibration amplitude of the top layer Zr(Y) atoms is strongly enhanced more than twice the bulk thermal vibration amplitude estimated from the simple Debye model. Such a low Debye temperature of the top surface is responsible for the strongly reconstructed surface structure with considerable O vacancies.

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