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A new model for $\sqrt{31} \times \sqrt{31}R9^\circ$ reconstruction of α -Al₂O₃ (001)
HAWOONG HONG, Argonne National Laboratory, AARON GRAY, TAI-C. CHI-ANG, University of Illinois, Urbana-Champaign — Research in oxides surface suffers reproducibility problems on its structure. However, $\sqrt{31} \times \sqrt{31}R9^\circ$ reconstructed α -Al₂O₃ (001) surface has been generated repeatedly by many different groups. This sapphire surface structure was known to be quite inert even to air exposure. The detailed structures have been studied with LEED, x-ray diffraction and AFM. The recent experimental studies conclude that the few topmost layers are composed of aluminum atoms and have metallic properties [1, 2]. Then a question arises why this surface seems to be inert to air exposure. Metallic aluminum is prone to oxidation according to theoretical investigation. Here we propose a new model for the $\sqrt{31} \times \sqrt{31}R9^\circ$ reconstruction involving oxidized top layers. For the direct structural information in the surface-normal direction, specular and non-specular crystal truncation rods were measured with x-ray diffraction. Only successful, if not perfect, fitting occurs with a dense top layer, which is reminiscent of oxidized aluminum (111) surface [3].

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