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Surface Structure of MBE-Grown α -Fe₂O₃(0001) by Intermediate-Energy X-ray Photoelectron Diffraction

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The surface structure of epitaxial α -Fe₂O₃(0001) grown on α -Al₂O₃(0001) has been investigated using intermediate-energy x-ray photoelectron diffraction. Comparison of experiment with quantum mechanical scattering theory reveals that the surface is Fe-terminated, and that the first four layer spacings are -41%, +18%, -8%, and +47% of the associated bulk values, respectively. These results agree reasonably well with the predictions of molecular mechanics and spin-density functional theory previously reported in the literature for the Fe-terminated surface. However, we find no evidence for an O-terminated surface predicted to be stable by spin-density functional theory.