

Surface X-ray Scattering Study of Fe-terminated Hematite (α -Fe₂O₃) (0001)

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Introduction: Iron oxides are important materials in catalysis [1] and photoelectrolysis [2]. Yet the atomic surface structures of iron oxides strongly influence their surface electronic and magnetic properties, there has been few experimental surface structure studies [3]. Also recent theoretical work predicted huge relaxations in first four layers for Fe-terminated α -Fe₂O₃(0001) surface [4].

Methods and Materials: We used surface X-ray scattering to study atomic structure of Fe-terminated α -Fe₂O₃(0001). Fe-terminated (1 \times 1) surface was prepared by Ar⁺ sputtering (500 eV) followed by sample annealing at 830 °C in oxygen pressure at 1×10^{-6} torr.

Results: Fig. 1 shows (101L) crystal truncation rod (CTR) with least square fitting of Fe-terminated surface. Contrary to previous studies [3] a good fit cannot be achieved with a model having simple relaxations of several top layers. Fitting was significantly improved after introducing 0.4 Å lateral displacements of the second layer oxygen atoms toward the third layer Fe atoms. Similar oxygen displacements have been observed in α -Al₂O₃(0001) surface [5]. Vertical deviations of atomic layers by -0.065, 0.660, -0.067, and 0.038 Å from ideal bulk lattice positions were obtained when going way from the Fe-terminated surface. Since the surface may have more complicating structure, direct method is underway to determine surface atomic structure.

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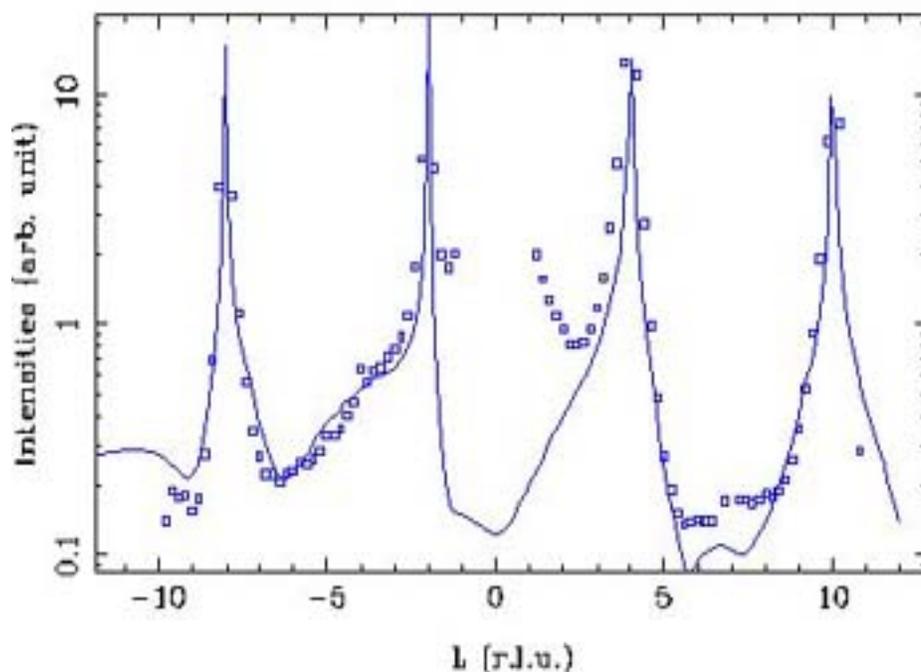


Fig. 1. (101L) crystal truncation rod of the α -Fe₂O₃(0001)-(1 \times 1) surface. Experiment momentum transfer, L, in reciprocal lattice units of the α -Fe₂O₃ lattice