PROBING THE LOCAL STRUCTURE OF ELECTROLUMINESCING RUTILE TIO2 WITH NEUTRON DIFFUSE SCATTERING AND ATOMISTIC MODELING

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The electroluminescing state of rutile TiO_2 is investigated via in-situ neutron diffuse scattering and atomistic modeling. This state is a new phase of matter created by applying a moderate E-field to a crystal and then very briefly heating it above room temperature. The crystal begins to glow and the structural, mechanical, and optical properties change drastically. Previous work suggests that an “avalanche” of Frenkel defects form during electroluminescence [1]. Modeling shows that these defects appear as “halos” around Bragg peaks in diffuse scattering (**c** in fig. 1). Our experiments show “needles” emanating from the Bragg peaks (**a** in fig. 1), inconsistent with a model including only Frenkel defects. Needles in reciprocal-space correspond to planar defects in real-space; we introduce “slip” defects with orientation perpendicular to the needles into our atomistic model (**d** in fig. 1) and reproduce the experimental diffuse scattering pattern (**b** in fig. 1). We show that these defects are responsible for the needle-like diffuse scattering pattern observed in experiment.

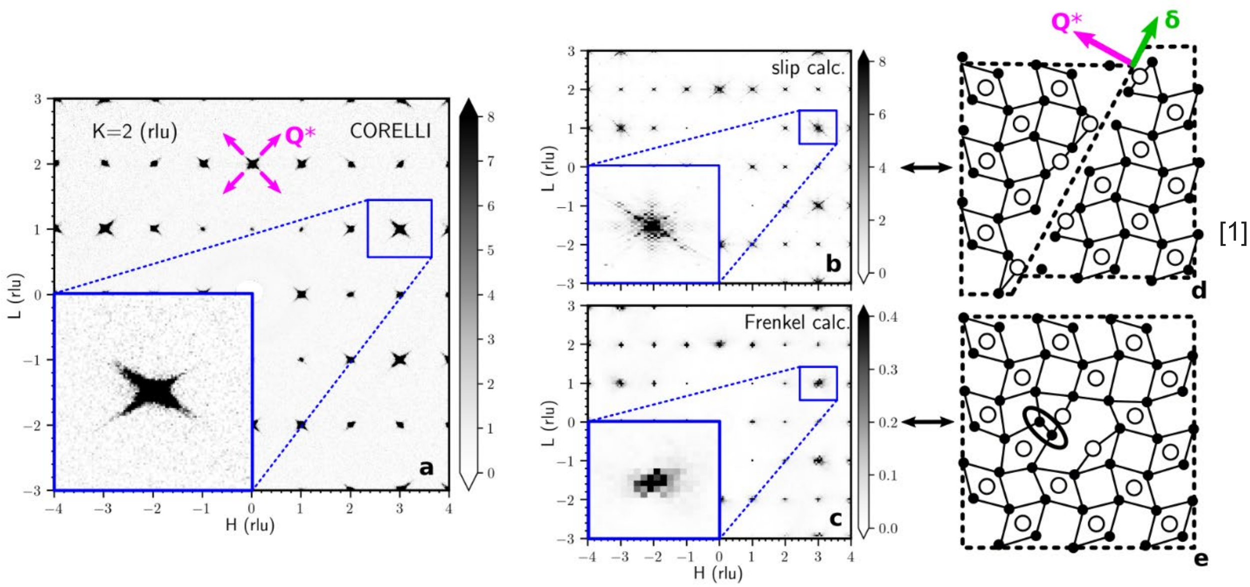

Figure 1 – a Diffuse scattering data measured on CORELLI at ORNL. b Calculated intensity with slip-defects. c Calculated intensity with Frenkel defects. d Cartoon diagram showing lattice distortions around a slip-defect. e Cartoon diagram showing lattice distortion around a Frenkel defect.

[1] Jongmanns, Malte, and Dietrich E. Wolf. "Element-specific displacements in defect-enriched TiO2: indication of a flash sintering mechanism." *Journal of the American Ceramic Society* 103.1 (2020): 589-596