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Forbidden Reflections in X-ray Crystal Truncation Rods: Using Surface Reference Waves to Distinguish Charge and Vibrational Asymmetry in Bulk Silicon[1] JESSE KREMENAK, YIYAO CHEN, SHAWN HAYDEN, MICHAEL GRAMLICH, PAUL MICELI, University of Missouri — X-ray reflections from diamond crystal structures with Miller indices that satisfy h+k+l = 4n+2, where n is an integer, are considered to be forbidden by crystal symmetry. However, asymmetry from valence charge distribution as well as anharmonic vibrations break the symmetry and result in non-zero intensity "forbidden reflections." Due to the absence of phase information, considerable effort, involving combined temperature-dependent x-ray and neutron scattering studies, was previously required to determine the contributions of charge and vibrations to these reflections. In the present work, we demonstrate that useful phase information can be gained in x-ray reflectivity and crystal truncation rod measurements where there is interference between waves scattered from the bulk and the surface. In this manner, surface reference waves can be used to determine the charge and vibrational asymmetry in the bulk crystal. These effects are demonstrated with in situ synchrotron x-ray scattering measurements on Si(111)7x7 surfaces with and without Ag films.

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