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Forbidden Reflections and Interference Effects in X-ray Reflectivity from Si(111)7x7¹ J.W. KREMENAK, YIYAO CHEN, S.T. HAYDEN, University of Missouri, M.W. GRAMLICH, University of Massachusetts Amherst, P.F. MICELI, University of Missouri — In diffraction, 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, these "forbidden reflections" have been observed experimentally, starting with W.H. Bragg over 90 years ago. Asymmetric charge distributions and anharmonic vibrations break the crystal symmetry and result in weak, but non-zero, intensities for these reflections. In the present work, we investigate the forbidden reflections in x-ray reflectivity and crystal truncation rods where we have discovered that the interference between bulk and surface waves can distinguish between the charge and vibrational origins of the reflections. Synchrotron x-ray scattering results, as well as a model, are presented. Understanding the properties of the forbidden reflections in diamond crystal structures not only provides greater insight into the crystal bonding and vibrations, but will also lead to better models for surface structures.

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