

Phonon and defect-induced effects in resonant "forbidden" reflections, V.E. Dmitrienko,^{a*} E.N. Ovchinnikova,^b K. Ishida,^c J. Kokubun,^c A. Kirfel,^d S.P. Collins,^e D. Laundy,^f A.P. Oreshko,^b Y. Joly^g and D. Cabaret^h,

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In this report, we present a survey of atomic displacement effects on the anisotropy of x-ray resonant scattering and discuss thermal-motion-induced (TMI) and point-defect-induced (PDI) "forbidden" reflections [1-5]. To this purpose, tensor structure factors and unusual polarization properties of both types of reflections are calculated. Owing to their resonant character, the TMI and PDI reflections allow for separate studies of both impurity and host atoms of different types. The considered phenomena can provide a very sensitive tool to assess point defects because only those atoms produce contributions to the PDI reflections that are "distorted" by defects and have appropriate absorption edges.

Strongly temperature dependent TMI reflections were recently observed in Ge [3,4] and in ZnO [5]. Owing to interference with the temperature-independent contribution, their intensities can increase and decrease with temperature. In Ge crystals, the contributions from vibrations parallel and perpendicular to atomic bonds were separated [4]. Drastic changes of the diffraction spectra were found in ZnO, contrary to the rather small changes observed for Ge. Using two different theoretical approaches [6,7] we present *ab initio* simulations of the temperature dependence and of diffraction spectra for Ge and ZnO.

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