Atomic Displacement Effects in Resonant 'Forbidden' Reflections

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In view of the very different x-ray and phonon energies it is rather surprising that phonons can drastically affect both the intensity and the spectrum of resonant scattering in crystals [1-5]. The reason is that resonant scattering is extremely sensitive, even to very small atomic displacements. Moreover, atomic displacements can change the symmetry of an atomic site, and thus induce an additional anisotropy of the atomic scattering factor near an absorption edge and therefore give rise to extra Bragg reflections, otherwise forbidden.

In this report, we present a survey of vibration effects on the anisotropy of x-ray resonant scattering and discuss thermal-motion-induced (TMI) and point-defect-induced (PDI) 'forbidden' reflections. To this purpose, tensor structure factors and unusual polarization properties of both types of reflections are calculated. Owing to their resonant character, 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.

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. 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 some simulations of the temperature dependence and of diffraction spectra for Ge and ZnO.

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