Thermal-Motion-Induced Forbidden Resonant Scattering: Experiment vs Theory

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The detailed simulations of forbidden reflections induced near the absorption edges by atomic motion are presented. The existence of such reflections, first predicted theoretically [1,2], is now well documented for Ge [3,4] and ZnO [5], see a detailed survey [6]. The reflections of this type can be also exited owing to the thermally independent dipole-quadrupole contribution [7]. The role of the temperature is to generate atomic displacements from the equilibrium sites and hence to provide the anisotropic terms of the tensorial atomic factor and to the structure factor. The numerical simulations were performed with the help of FDMNES, PARATEC and XKDQ codes, which allowed fitting the results both for Ge and for ZnO.

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