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S E M I N A R

aus

Halbleiterphysik und Nanotechnologie

Di, 14.5.2013, 14:15 Uhr
Hörsaal für Physik

"Bulk dipole contribution to second harmonic generation in diamond lattices"

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The recent high interest in surface science techniques capable to probe surfaces in-situ has renewed the interest in linear and nonlinear optical techniques such as second harmonic generation (SHG). This interest has been accompanied by theoretical efforts to model the measured data, interpreting them either in a classical picture or taking into account quantum mechanics by involving transitions between initial and final states. Especially for SHG the interpretation and the origin of the data is controversial. Some authors claim that part of the SHG response arises from the surface and bulk quadrupoles or from magnetic dipole effects, whereas others are mainly considering surface contributions. To our knowledge, however, all the literature has up to now neglected bulk dipole transitions in materials with inversion symmetry using the following argument: Materials with inversion symmetry are described by potentials with even powers of the coordinates (i.e. $\propto r^2$, $\propto r^4$, etc.). and so only odd forces can result.

I have developed a different point of view: Si(111), respectively its atoms, can be described in a simple picture by four equivalent covalent bonds with a sequence of layers, which are alternatingly bound by one up bond or by three down bonds to the next layer. For the case of normal incidence, because the exciting field decays along z due to absorption when penetrating into the bulk, the nonlinear radiation of the higher lying Si(1) atom is not fully canceled by the radiation of the deeper in the bulk positioned atom Si(2), because this atom experiences a lower field. So, in the antenna picture for the Si(111) case the two waves, originating at Si(1), respectively Si(2) do not fully destructively interfere. Finally I propose an experiment, exploiting the different dispersion for the fundamental as well as frequency doubled radiation to determine this effect.