

Influence of Random Internal Fields on the Tunneling of Point Defects in Alkali Halide Crystals

R. Kühn, M. Thesen

Institut für Theoretische Physik, Universität Heidelberg, D-69120 Heidelberg, Germany

S. Ludwig, C. Enss

Kirchhoff-Institut für Physik, Universität Heidelberg, D-69120 Heidelberg, Germany

Alkali halide crystals doped with certain impurity ions show a low temperature behaviour, which differs significantly from that of pure crystals. The origin of these characteristic differences are tunneling centers formed by atomic or molecular impurity ions. The low energy excitations arising from these tunneling systems dominate the thermal, acoustic and dielectric response of such crystals at low temperatures. In the limit of low concentrations, interactions among the defects can be neglected and the tunneling centers can be considered as approximately independent. In this case, the physics of such states can be described theoretically from a microscopic point of view which is based upon the tunneling motion between localized pocket states. Isolated hydroxyl ions in NaCl possess six equivalent potential minima along the $\langle 100 \rangle$ crystal directions, between which they reorient via tunneling at low temperatures. The tunneling motion partially lifts the sixfold degeneracy of the ground state, leading to three energy levels with degeneracies 1-3-2. We have investigated the dielectric susceptibility of hydroxyl ions in NaCl crystals at very low concentrations (below 30 ppm). We find that the temperature dependence of the susceptibility is noticeably different from what one would expect for isolated defects. The origin of these deviations lies in the influence of random internal strains arising from imperfections of the host crystal. While on a phenomenological basis this is simple to understand, a quantitative description is involved, because of the level scheme of these tunneling defects. We will present the experimental data and a theoretical model which allows a quantitative understanding on a microscopic basis.