Experimental measuring and numerical calculations of vibrations associated with Ni charged impurities in ZnSe:Ni.

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In previous works the repetitions of the zero phonon line of Ni impurity excitons of ZnSe:Ni crystals have been analyzed in one phonon region. The purpose of the present work is to analyze the multiphonon repetitions detected in modulation electroabsorption spectra on the basis of modelling of a crystal lattice dynamics of $ZnSe:Ni^{+1}$ and $ZnSe:Ni^{+3}$ crystals. The experimental electroabsorption spectra of ZnSe crystals doped with Ni in various charge states were taken at temperature 4.2K. The electroabsorption spectrum of a Ni acceptor exciton in ZnSe:Ni consist of approximately more than 20 zero phonon line intensive repetitions. The observed spectra show an unusual combination repetition structure which may be qualitatively recognized as the results of a photoinduced distortion near an Ni impurity center charged positively Ni^{+3} or neqatively Ni^{+1} with respect to the lattice.

For the understanding of the structure of vibration repetitions the calculations of the lattice vibrations for ZnSe:Ni have been performed with an account of change of the Ni impurity charge state due to photoionization of an Ni impurity. A recursive technique in a shell model was used for modelling of the lattice dynamics. The calculations have been carried out with the account of coulomb interaction for a cluster containing about 1000 ions. The lattice relaxation near the charged Ni impurity under consideration was also taken into account. The localised vibration frequencies for A_1, E and T_2 symmetry modes have been obtained.

Our experimental results and model calculations are perhaps the first manifestations of the fact that a significant anharmonicity is an inherent property of lattice vibrations induced by impurities charged with respect to the lattice.