THE EFFECT OF UNIAXIAL STRESS ON THE OFF-CENTER POTENTIAL OF CU^+ AND AG^+ DEFECTS IN ALKALI HALIDE CRYSTALS

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Odd parity lattice distortions near Cu^+ and Ag^+ defect ions on normal lattice sites in alkali halide crystals mix electronic defect states of different parity and give rise to a noticeable oscillator strength of the parity-forbidden electric dipole transitions $ns^1S_0 \rightarrow np^1P_1$ ($n = 3$ for Cu^+, $n = 4$ for Ag^+) in the UV-spectral range. In this way the intensity of the absorption bands indicates the behaviour of the local lattice distortions under extranious fields or at different temperatures and enables us to study the potential of the defect ion. Here we report on the effect of uniaxial stress on the potential of Cu^+ in KCl and Ag^+ in rubidium halides, where the small defect ion shifts from the symmetry center of the lattice cell to an off-centre position.

For sufficiently large off-center distortions the defect potential can be approximated by a number of separated and symmetrically arranged potential wells with high walls between them (1). We describe the defect displacement from the symmetry center by the symmetry coordinate $\vec{Q}_4$ which transforms as a vector under the elements of the point group O_h. The relevant odd-parity term of the electron-lattice interaction for the defect ion in the n-th potential well is given by:

$$H'_{el} = \sum_{i=1}^{3} V_{4i} \left\{ Q^-_{4in} + Q^-_{4i} \right\} \qquad [1]$$

where $\vec{Q}_{4n}^-$ is the static displacement of the defect ion and $\vec{Q}_4^-$ describes vibrational distortions of the symmetry Γ_4^-. For the oscillator strength of a parity forbidden electric dipole transition from the ground state $|j^+\rangle$ to the excited state $|k^+\rangle$ we obtain by using perturbation theory:

$$f_{j\to k} = \sum_n \frac{e^{-\frac{E_n}{kT}}}{\sum_n e^{-\frac{E_n}{kT}}} \cdot \sum_{l,m=1}^{3} B_{lm}(j,k)\,(Q_{4ln}^- Q_{4lm}^- + \langle Q_{4l}^- Q_{4m}^- \rangle) \qquad [2]$$

The Boltzmann-factor considers the occupation probability of the n-th potential well with minimum energy E_n. The first term of [2] is due to static off-center distortions, the second term describes the the component of the oscillator strength which is due to vibrations. $\langle\ \rangle$ means the thermal average.

Uniaxial stress affects the oscillator strength [2] in three different ways: First the off-center elongation $\vec{Q}_{4n}^-$ of the defect ion in the stressed crystal depends on the projection of $\vec{Q}_{4n}^-$ on the stress axis, and secondly the frequency ω of the "odd" mode in a single well may split (1),(2). Here we report on the change of the

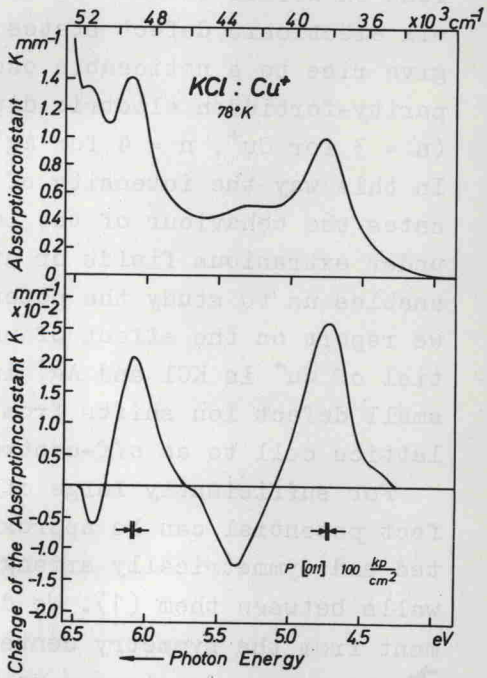

Fig.1. Difference of absorption constant of KCl:Cu^+ for light polarized parallel and perpendicular to the stress axis.