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OFF-AXIS CONFIGURATION OF F_A (Li) CENTRES IN KF

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Abstract: The off-axis configuration of F_A dipoles was identified in KF:Li⁺. The centre tilt from the crystal axis is, as expected, larger in KF:Li⁺ than in KCl:Li⁺ and in RbCl:Li⁺.

1. Introduction

The off-centre displacement of Li⁺ ions in crystals of alkali halides, showing a sufficiently large lattice parameter, was experimentally observed in KCl [1] and in RbCl [2], and theoretically calculated for several systems [3]. Such a peculiar configuration of the isolated impurity seems to be correlated in the above systems to a tilt from the crystal axis of the F_A dipole, formed by association of the impurity ion with a nearest-neighbour anion vacancy trapping an electron. The off-axis deviation of the F_A (Li) centres was quantitatively determined both in KCl:Li⁺ [4] and RbCl:Li⁺ [5] by means of optical measurements. In this work the investigation on the configuration of F_A (Li) dipoles is extended to KF:Li⁺.

2. Experimental results and discussion

The technique used for studying the off-axis geometry of the F_A (Li) centres is the analysis of their photostimulated reorientation under polarized optical pumping into the range of the F_A absorption [6]. The alignment process was theoretically treated, by taking into account both the off-axis effect of the dipoles and the overlap of the two F_A absorption bands, for experiments in equilibrium conditions [4] or during transient phenomena [7].

In KF:Li⁺ preliminary absorption measurements have been performed on transient effects. After thorough orientation of the centres by irradiation with monochromatic F_A light polarized along one of the crystal axes, the polarization plane of the incident beam was suddenly rotated: as a consequence, a depopulation occurs for centres lying parallel to the above direction, while the centre population along perpendicular directions increases correspondingly. The initial absorption $\alpha(0)$ and the steady-state absorption $\alpha(\infty)$, measured for two different rotations of the polarization plane of the exciting light (Figure 1),

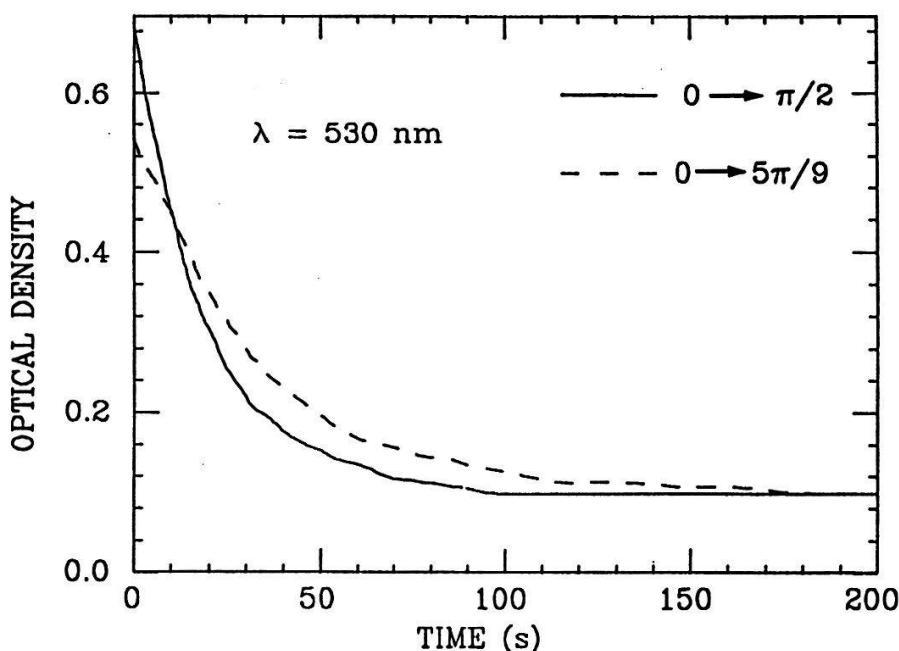


Figure 1: Kinetics of the $F_A(Li)$ centre photostimulated reorientation in $KF:Li^+$ at 77 K.

allow the calculation of both the off-axis angle θ of the F_A dipoles and the ratio R of the cross sections related to the two F_A transitions.

From these and other results, obtained at various wavelengths of the pumping light, it is possible to deduce a first approximate evaluation of θ in $KF:Li^+$, which is slightly bigger than 10° . Such value, to be confirmed by luminescence experiments at various temperatures, is larger than those in $KCl:Li^+$ and in $RbCl:Li^+$, as expected because of the more pronounced displacement of the isolated Li^+ ion in this system [3].

3. References

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