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Autor: Scacco, A. / Somma, F. / Rossi, M.
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OFF-AXIS CONFIGURATION OF $F_A(\text{Li})$ CENTRES IN KF

A. Scacco, F. Somma, M. Rossi, F. De Matteis, Dipartimento di Fisica, Università *La Sapienza*, P.le A. Moro 2, 00185 Roma, Italy

G. Baldacchini, ENEA, Dip.TIB, U.S. Fisica Applicata, CRE Frascati, C.P.65, 00044 Frascati, Italy

U.M. Grassano, Dipartimento di Fisica, Università di Roma-Tor Vergata, V. O. Raimondo, 00173 Roma, Italy

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

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 $F_A(\text{Li})$ centres was quantitatively determined both in $\text{KCl}:\text{Li}^+$ [4] and $\text{RbCl}:\text{Li}^+$ [5] by means of optical measurements. In this work the investigation on the configuration of $F_A(\text{Li})$ dipoles is extended to $\text{KF}:\text{Li}^+$.

2. Experimental results and discussion

The technique used for studying the off-axis geometry of the $F_A(\text{Li})$ 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 $\text{KF}:\text{Li}^+$ 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),

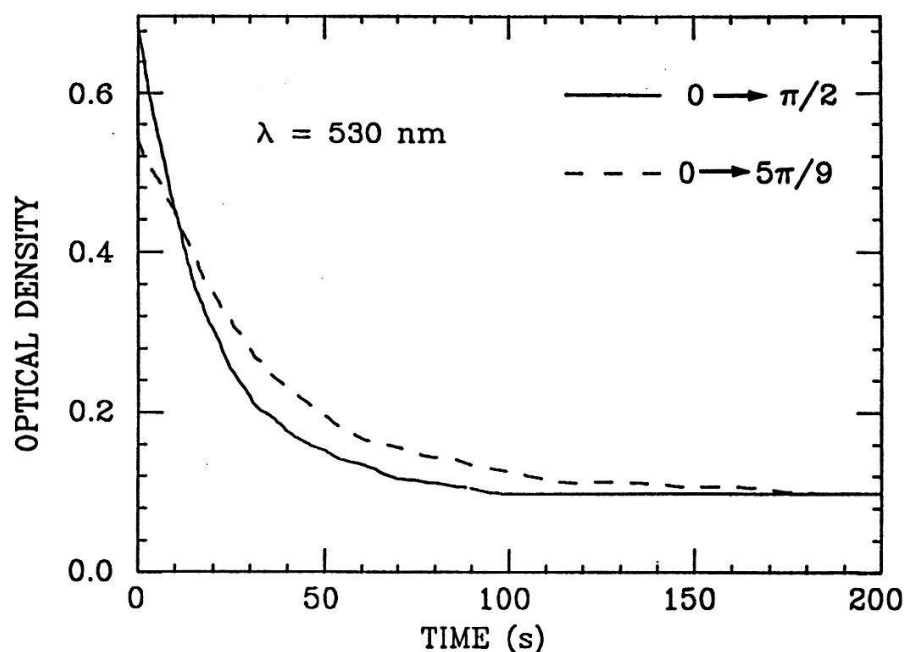


Figure 1: Kinetics of the $F_A(\text{Li})$ centre photostimulated reorientation in $\text{KF}:\text{Li}^+$ at 77 K.

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 $\text{KF}:\text{Li}^+$, which is slightly bigger than 10° . Such value, to be confirmed by luminescence experiments at various temperatures, is larger than those in $\text{KCl}:\text{Li}^+$ and in $\text{RbCl}:\text{Li}^+$, as expected because of the more pronounced displacement of the isolated Li^+ ion in this system [3].

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