Electric-Field-Induced Orientation of Iron Tetragonal Centers in KTaO₃

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Abstract—Fe³⁺–O²⁻ impurity centers in a KTaO₃ sample to which a dc electric field \( E = 75 \) kV/cm is applied are shown to be oriented at temperatures \( T \geq 120 \) K. In these conditions, the effective local field acting on the electric dipole moment of a center exceeds the applied field by a factor 7.6. © 2000 MAIK “Nauka/Interperiodica”.

1. The orientation of defect centers in a lattice can be ordered by exerting an anisotropic action on the crystal. The alignment of Fe³⁺–O²⁻ tetragonal centers in a KTaO₃ cubic crystal by polarized light was discovered [1] and studied in considerable detail [2]. The mechanism of this alignment was shown [2] to consist in anisotropic recharging of the centers by polarized light, which does not involve their real reorientation.

By a universally accepted model [3, 4], the center being discussed here represents a complex of an impurity ion Fe³⁺ at a K⁺ site and an O²⁻ ion occupying an interstitial site located near Fe³⁺ along one of the \( \langle 100 \rangle \) crystallographic directions. Thus, the KTaO₃ lattice allows six possible center orientations (Fig. 1).

Because the center being discussed has an electric dipole moment (Fig. 1), one may attempt to order the orientation of the Fe³⁺–O²⁻ centers by a method different from the one employed in [1, 2], namely, by applying a dc electric field to the sample. It is known that, for a dipole center to be oriented by an external electric field, it must have a possibility to undergo spontaneous (thermal) reorientation at the temperature of the experiment. Recent publications [5] suggested the existence of such reorientations of this center at the temperature \( T = 117–120 \) K and reported determination of the barrier separating the interstitial positions of the O²⁻ ion (0.34 ± 0.02 eV).

This work reports on the orientation of the Fe³⁺–O²⁻ complexes in KTaO₃ by an external electric field.

2. The study was made on KTaO₃: Fe single crystals grown from a batch containing 20000 ppm iron at the Physical Department of the Osnabrück University, Germany. Rectangular samples with the edges aligned with \( \langle 100 \rangle \) and measuring typically \( 0.7 \times 2 \times 3 \) mm were cut from a single-crystal boule and studied in the as-grown state. Silver-paste electrodes were applied to \( 2 \times 3 \) mm faces.

EPR spectra were measured with a standard SE/X 2544 X-range spectrometer, with the samples held in liquid nitrogen or in a jet of its vapor. In the latter case, the temperature was stabilized to within \( ±1 \) K.

The electric fields used in experiments in both liquid and gaseous nitrogen were up to 150 kV/cm.

3. The optical alignment of Fe³⁺–O²⁻ centers by polarized light was observed to set in at \( T = 78 \) K [1, 2]. This method of ordering of the center orientation is obviously more efficient, the lower the probability of thermal reorientation of the center at the temperature of

**Fig. 1.** Fe³⁺–O²⁻ center in a KTaO₃ lattice (in one of its six possible orientations). In Figs. 2 and 3, the field \( E \) is applied along \( [010] \), and the field \( H \) is canted from \( [010] \) by angles \( \theta_1 \) and \( \theta_2 \), respectively.
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The experiment. At $T = 78$ K, the degree of the light-induced center alignment persists indefinitely in the dark; that is, thermal reorientation does not occur at this temperature at all. On the other hand, as already mentioned, in order for an external electric field to be capable of orienting a center, thermal reorientation must be allowed. It thus becomes clear that no orientation of the Fe$^{3+}$–O$_{2}^{2–}$ centers in an external electric field should take place at $T = 78$ K, and that higher temperatures are required for it to be observable.

The experiments carried out confirmed these arguments. Figure 2 shows an EPR line corresponding to centers with the tetragonal axis aligned with $[010]$; the line was obtained at $T = 78$ K in a field $E = 92$ kV/cm applied along the axis of the above centers. (The $H$ field made an angle $\theta_1 = 18^\circ$ with the tetragonal axis of the centers, an orientation corresponding to the maximum line splitting of this center [6].) The line is seen to split in two equal components, with the splitting (19 Oe) being as large as twice the original linewidth. Thus, at $T = 78$ K, the number of the centers with the dipole moment directed along the field is equal to that of the centers with the dipole moment oriented opposite to the field, and it persists indefinitely. This means that, at $T = 78$ K, an external electric field does not orient the centers (although, as this will be shown in Section 4, in these conditions $pE_{loc}/kT > 4$, where $E_{loc}$ is the effective local field acting on the center dipole); i.e., the centers do not undergo thermal reorientation at this temperature.

Experiments with an electric field performed at higher temperatures revealed reorientation of the centers starting from $T \approx 120$ K. It was found that quantitative measurements of the extent of orientation can be more conveniently carried out by comparing the intensities not of the components of the field-split line, but rather those of the lines corresponding to the center orientation along different $[100]$ axes. We used the magnetic-field orientation with $H$ canted by 1–2° in the (001) plane from the $[110]$ direction; in this case, one observes two lines near $H = 1500$ Oe (Fig. 3a): one of the lines corresponds to two centers with the tetragonal axis along $[110]$, parallel to $E$, and the other is associated with two other centers with their axis along $[100]$, perpendicular to $E$.

Figure 3 shows characteristic recordings of these two lines obtained at $T = 122$ K in zero field and in fields of 47 and 75 kV/cm after having kept the sample in the field for a long time. The integrated-intensity ratio of these two lines obtained at 75 kV/cm differs by about four times from that measured in zero field. Estimation of the degree of alignment as $\eta = (I_0 - I_\perp)/(I_0 + I_\perp)$, where $I_0$ and $I_\perp$ are the intensities of the two lines, yields $\eta = 0.6$. Thus, the existence of thermal reorientation of the center under study at $T = 122$ K cannot be questioned.