

Temperature dependence of the photoconductivity of color centers

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As is well known, the abrupt decrease in photoconductivity with a lowering of the temperature (as a rule, at $T \leq 150\text{K}$) when alkali-halide crystals with color centers are irradiated with F -band light is due to the transition of an electron to an excited state from which a transition to the conduction band is possible only as a result of additional thermal excitation.¹ The thermal-activation energy ΔE which appears in the expression for the low-temperature asymptotic form of the photoconductivity

$$\sigma \sim \exp(-\Delta E/T), \quad (1)$$

was measured experimentally some time ago for a number of ionic crystals (see, e. g., Ref. 2). No reliable theoretical method of calculating this quantity has existed thus far.

The quantity ΔE in (1) can be calculated if we allow for the fact that as a result of phototransition an F -center electron relaxes to the first self-consistent state.³ Table I gives the values obtained in Ref. 3 for the total energies

TABLE I

Substance	$\tilde{\epsilon}$	μ/m	J_1 , eV	ΔE_T , eV	ΔE_{exp} , eV
KCl	3.93	0.922	0.262	0.173	0.154
KBr	4.54	0.700	0.180	0.130	0.135
KI	5.92	0.536	0.119	0.097	0.110
RbCl	3.9	1.03	0.267	0.17	0.18

Note: The experimental values of μ/m , obtained by the cyclotron-resonance method, are taken from Ref. 5.

J_1 of an electron in the first self-consistent state and the experimental values of ΔE for a number of substances.¹ In calculating ΔE we must allow for the fact that the relaxed excited state dissociates thermally to a free polaron state:

$$|\Delta E| = |J_1| - |E_p|, \quad E_p = -0.0543 \mu e^4 / \hbar^2 \tilde{\epsilon}^2, \quad (2)$$

where for E_p we have taken the asymptotic value obtained in the tight-binding limit.⁴ As follows from Table 1, the values ΔE_T calculated from formula (2) are close to the experimental values ΔE_{exp} .

The results can be used to calculate quantities for which experimental values are not available at present. Thus, e.g., the experimental value of the thermal-activation energy of rock salt is $\Delta E_{\text{exp}}(\text{NaCl}) = 0.074$ eV (Ref 2.) The total energy in the first self-consistent state for NaCl is $J_1 \approx 0.12 e^4 \mu / \hbar^2 \tilde{\epsilon}^2$, where $\tilde{\epsilon} = 3.82$. Then from (2) we get

$$\mu/m (\text{NaCl}) \approx 7.61 \Delta E_{\text{exp}} \tilde{\epsilon}^2 / R \approx 0.6, \quad (3)$$

where R is the Rydberg constant. A similar calculation carried out for RbBr ($\Delta E_{\text{exp}} = 0.16$ eV, $\tilde{\epsilon} = 4.35$, $J_1 \approx 0.17 e^4 \mu / \hbar^2 \tilde{\epsilon}^2$) gives $\mu/m \approx 0.96$.

In conclusion, we point out that, strictly speaking, the expression (1) represents not the photoconductivity but the low-temperature asymptotic form of the quantum yield. In the very simple version of photoconductivity theory considered here the expression (1) takes no account of the mobility contribution, which is insignificant for most crystals (neglect of this contribution can result in an error amounting to 10-15% of ΔE). This, together with the use of approximate values of E_p and J_I (which are valid only in the limit of strong electron-phonon coupling), explains the slight difference between the experimentally measured and calculated values considered here.

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