SOVIET PHYSICS JETP VOLUME 6 (33), NUMBER 3 MARCH, 1958

OPTICAL PROPERTIES OF F^- CENTERS

V. L. VINETSKII

Submitted to JETP editor March 27, 1957

J. Exptl. Theoret. Phys. (U.S.S.R.) **33**, 780-787 (September, 1957)

The quantum states are considered for a system consisting of a crystal with two opposite charge vacancies spaced a distance of half a lattice period from each other and of an electron which interacts with the optical vibrations of the crystal localized near this pair of vacancies (crystal with F^- center). The problem is solved in the macroscopic approximation. The parameters of the self-consistent ground state of the system are calculated. The frequencies and absorption coefficients of light are calculated in the Franck—Condon approximation for photo-transitions to the lowest excited states. The azimuthal dependence of the degree of polarization of luminescence due to irradiation with polarized light in the F^- absorption bands is also computed; this dependence may be used to identify the F^- centers. The results are carried to numerical values for the KCl crystal.

IN the present work it is shown that in the macroscopic approximation a system comprising a crystal plus a pair of opposite charge vacancies plus an electron (a crystal with an F^- center) is energetically more favorable than a system comprising a crystal plus an F^- center (Sec. 1). Although the gain is not large — on the order of hundredths of an electron volt — the result obtained furnishes the basis for assuming that under favorable conditions a sufficiently large concentration of F^- color centers can exist in a crystal. A temperature sufficiently low so that the mobility of the vacancies is small and the F^- centers are not decomposed by thermal fluctuations must be considered as a necessary condition for the presence of stable F^- centers. The formation of F^- centers can occur, for example, directly on coloration of a crystal when electrons are located at vacancy pairs, the concentration of which in a crystal can be comparable to the concentration of discrete vacancies and even significantly exceed the latter (if the crystal is maintained for a sufficient time, for example, at room temperature).[1] Another possibility of obtaining F^- centers can be connected with the decomposition of more complex color centers (for example M centers).

An examination of the properties, particularly the optical properties of a crystal containing F^- color centers thus appears desirable.

1. THE GROUND STATE OF A CRYSTAL WITH AN F^- CENTER

In the macroscopic approximation using methods developed by Pekar,[2] the energy of the system crystal + F^- center can be written in the form

$$\hat{H} = -\frac{\hbar^2}{2\mu}\Delta + e\int\frac{(\mathbf{r}_1-\mathbf{r})P(\mathbf{r})}{|\mathbf{r}_1-\mathbf{r}|^3}\,d\tau + \frac{e^2}{\varepsilon}\left(\frac{1}{r_c}-\frac{1}{r_a}-\frac{1}{R}\right) + {}^1/_2\sum_k \hbar\omega_k\left(q_k^2-\frac{\partial^2}{\partial q_k^2}\right). \tag{1}$$

Here the first term represents the kinetic energy of the electron, the second — the energy of interaction of the electron with the polarized surroundings, the third — the energy of electrostatic interactions of the electron with the positive (a) and negative (c) vacancies and the vacancies with one another; the fourth — the energy of normal lattice vibrations; μ is the effective mass of the electron: $\mathbf{P}(\mathbf{r})$ is the inertial part of the specific polarization of the crystal brought about by the field of the electron; ϵ is the dielectric constant of the crystal; r_a and r_c are the distances from the electron to the vanancies a and c, R is the distance between the vanancies, ω_k and q_k are the frequencies and normal coordinates of the polarization oscillations of the crystal.

Instead of solving the Schrödinger equation with the Hamiltonian (1) it is more convenient to find the minimum of the corresponding functional. If, as in Refs. 3 — 5, one disregards the dependence of R on q_k and selects an approximating function to the system in the multiplicative form

$$\Psi = \psi(r)\,\Phi(\ldots q_k\ldots), \tag{2}$$

then as a result of minimizing over $\Phi(\ldots q_k \ldots)$ the energy of the system can be written down in the following manner:

$$\overline{H} = J[\psi(r)] + \sum_k \hbar\omega_k (n_k + 1/2), \tag{3}$$

where n_k are quantum numbers of the oscillators which describe the vibrations of the lattice and J is a functional which depends only on the electronic part of the wave function of the system

$$J[\psi(r)] = \frac{\hbar^2}{2\mu}\int (\nabla\psi)^2 \, d\tau - \frac{e^2}{\varepsilon}\int \frac{\psi_a^2}{r_a}\, d\tau - \frac{e^2 c}{2}\int \frac{\psi^2(1)\,\psi^2(2)}{r_{12}}\, d\tau_{12} + \frac{e^2}{\varepsilon}\int \frac{\psi^2}{r_c}\, d\tau - \frac{e^2}{\varepsilon R}. \tag{4}$$

Here c is the well-known parameter of polaron theory.[2] The first three terms in Eq. (4) represent the corresponding functional of the F center formed at the vanancy a.

Further, the variation of J [ψ] with respect to $\psi(r)$ must be carried out.

The mean value of the intensity of the electric field set up by a vacancy c in the region where the electron of an F center a is localized is equal to

$$\overline{E} = \int \psi^*(r) \frac{e^2}{\varepsilon r_c^2} \psi(r)\, d\tau,$$

which in real crystals, as calculation shows, is some 10 — 20 times smaller than the mean value of the intensity of the electric field produced by the vacancy a. One can assume, therefore, that the effect of the electric field of the vacancy c leads to a small change of the wave function of the ground state of the F center which has, according to Ref. 2, the following form

$$\psi_0(r) = (7\pi)^{-1/2}\alpha^{3/2}(1 + \alpha r_a)\, e^{-\alpha r_a}. \tag{5}$$

Two different approximations of the electronic part of the wave function of the ground state of the system which take into account such a change have been tested:

(a) $\psi(r)$ is approximated by a wave function of the form Eq. (5) whose maximum is located at some point b which, generally speaking, does not coincide with point a:

$$\psi_0(r) = (7\pi)^{-1/2}\alpha^{3/2}(1 + \alpha r_b)\, e^{-\alpha r_b}. \tag{6}$$

From symmetry considerations it follows that the point b must lie on the axis ac. The distance between the vacancy a and the point b (denoted by ρ) and the reciprocal radius of the state of the electron α are the parameters of the approximation. It is more convenient to use the quantities $t = \rho/R$ and $x = \alpha R$ as the independent parameters. Substituting Eq. (6) in Eq. (4) assuming $t \ll 1$ and confining ourselves to terms of second order of smallness we arrive at a functional which depends on t and x:

$$J[t, x] = \frac{\hbar^2}{2\mu R^2}\frac{3}{7}x^2 - \frac{e^2}{14\varepsilon R}x\left(9 - \frac{4}{3}x^2 t^2\right) + \frac{e^2}{14\varepsilon R}[\varphi_0(x) + t\varphi_1(x) + t^2\varphi_2(x)] - \frac{e^2 c}{2R}0.428\,x - \frac{e^2}{\varepsilon R}, \tag{7}$$

where

$$\varphi_0(x) = 14 - e^{-2x}(14 + 19x + 10x^2 + 2x^3), \qquad \varphi_1(x) = -14 + e^{-2x}(14 + 28x + 28x^2 + 16x^3 + 4x^4),$$
$$\varphi_2(x) = 14 - e^{-2x}(14 + 28x + 28x^2 + 20x^3 + 12x^4 + 4x^5). \tag{7a}$$

Minimizing Eq. (7) over t permits, as a result of simple transformations, writing the functional in the form

$$J[x] = \frac{e^2}{\varepsilon R}\left\{-1 + \frac{1}{14}\left[\frac{\hbar^2\varepsilon}{\mu e^2 R}3x^2 - 3(\varepsilon c + 3)x + \varphi_0(x) - \frac{3\varphi_1^2(x)}{4[3\varphi_2(x) + 4x^3]}\right]\right\}.$$

Minimizing J [x] over x permits calculation of the parameters of the self-consistent ground state of the system. Calculations carried out for a series of alkali-halide crystals show that $J(x_{\min})$ is approximately 0.01 — 0.02 ev lower than the corresponding values obtained for the F center. In particular, for the KCl crystal ($\epsilon = 4.78$, $c = 0.25$, $R = 3.14$ A) the values $J = -2.19$ ev, $t = 0.043$, and $x = 4.73$ are obtained.

(b) As the approximating function we use the function proposed by Perlin[6]

$$\psi(r) = (1 - 1/2\,\lambda^2)\,\psi_0(r) + \lambda\varphi(r), \tag{8}$$

where $\lambda \ll 1$; $\psi_0(r)$ is determined by Eq. (5), and

$$\varphi(r) = \pi^{-1/2}\gamma^{5/2}e^{-\gamma r}\, r\cos\theta. \tag{9}$$

Substitution of Eqs. (8) and (9) in Eq. (4) leads to a functional which depends on λ, x and $\omega = \gamma/\alpha$:

$$J[\lambda, x, \omega] = (e^2/\varepsilon)(a_0 + \lambda a_1 + \lambda^2 a_2 + \ldots), \tag{10}$$

$$a_0 = \frac{1}{14R}\left[\frac{3\hbar^2\varepsilon x^2}{\mu e^2R^2} - G_0(x) - 3\varepsilon cx\right],$$

$$a_1 = \frac{1}{R}\frac{8}{\sqrt{7}}\frac{\omega^{5/2}}{(1+\omega)^6}\frac{1}{x}\{8(6+\omega) - e^{-x(1+\omega)}[x^4(1+\omega)^4$$

$$+ x^3(1+\omega)^3(7+\omega) + 4x^2(1+\omega)^2 + 8x(1+\omega)(6+\omega) + 8(6+\omega)]\},$$

$$a_2 = \frac{1}{14R}\left\{\frac{\hbar^2\varepsilon}{\mu e^2R}x^2(7\omega^2-3) + G_0(x) - \frac{7}{x^2\omega^2}[\omega^3x^3 - 2\omega^2x^2 - 6 + e^{-2x\omega}(6 + 12\omega x + 14\omega^2x^2 + 11\omega^3x^3 + 6\omega^4x^4 + 2\omega^5x^5)]\right.$$

$$\left. + \varepsilon cx\left[-1 + \frac{\omega^4}{(1+\omega)^7}(66 + 84\omega + 40\omega^2 + 7\omega^3) - \frac{8}{3}\frac{\omega^5}{(1+\omega)^9}(297 + 126\omega + 14\omega^2)\right]\right\},$$

$$G_0(x) = 9x - 14 + e^{-2x}(14 + 19x + 10x^2 + 2x^3). \tag{11}$$

Disregarding terms of order λ^3 and higher, we determine λ from the condition $\partial J/\partial\lambda = 0$; substituting the value of λ obtained in this way in Eq. (10) we obtain

$$J[x, \omega] = (e^3/\varepsilon)(a_0 - a_1^2/4a_2). \tag{12}$$

Setting $x = x_0 + \zeta$ where $x_0 = \alpha_0 R$, (α_0 is the reciprocal radius of the state of the electron of the F center) assuming $\zeta \ll 1$ and varying J over ζ, it is possible to obtain a functional which depends only on ω. In view of its unwieldiness, the analytical expression for $J[\omega]$ is not quoted. Minimizing J over ω can be carried out graphically. As a result we obtain the values of J_0 and of the parameters of the approximation ω, ζ, and λ. For the KCl crystal the calculation leads to the following values of the parameters of the self-consistent ground state of the system: $J_0 = -2.21$ ev, $\lambda = -0.13$, $\zeta = -0.13$, and $\omega = 0.70$. The value of J_0 for the F center in KCl, according to Ref. 2, amounts to -2.17 ev.

The calculations carried out above show that the deformation of the wave function of the ground state of an F center which occurs under the influence of the electric field of a nearest neighbor vacancy is actually small and leads to a lowering of the energy of the system by 1 — 2% (hundredths of an ev).

2. EXCITED STATES OF THE F⁻ CENTER

The excited states of the F⁻ center will be examined below in the Franck-Condon approximation. The results of the preceding section permit the choice of the wave function of the F center Eq. (5) for the wave function of the ground state of the system. In this case the Schrödinger equation can be written in the form

$$E\psi = \left\{-\frac{\hbar^2}{2\mu}\Delta - \frac{e^2}{\varepsilon r_a} + \frac{e^2}{\varepsilon r_c} - \frac{e^2c}{r_a}\left[1 - e^{-2\alpha r_a}\left(1 + \frac{19}{14}\alpha r_a + \frac{5}{7}\alpha^2r_a^2 + \frac{1}{7}\alpha^3r_a^3\right)\right]\right\}\psi. \tag{13}$$

This equation has been solved by means of perturbation theory. The term $W = e^2/\epsilon r_c$ was taken as a perturbation, whereby the Hamiltonian of the system in the zeroth approximation coincides with the Hamiltonian of the F center. The energy terms of the F⁻ center in the first approximation of perturbation theory are determined from the secular equation, taking into account four levels of the F center E_1^0, E_2^0, E_3^0 and E_4^0, which correspond to the states $2p_0$, $2s$, $2p_1$ and $2p_{-1}$. We present below the values of the energies and the wave functions of the lowest excited states of the F⁻ center in first order perturbation theory:

$$\begin{gathered}
E_1 = {}^1\!/_2(E_1^0 + E_2^0 + W_{11} + W_{22}) - \sqrt{{}^1\!/_4(E_1^0 - E_2^0 + W_{11} - W_{22})^2 + |W_{12}|^2},\\
\psi_1 = A(\varphi_{2p_0} + c_1\varphi_{2s}),\\
E_2 = {}^1\!/_2(E_1^0 + E_2^0 + W_{11} + W_{22}) + \sqrt{{}^1\!/_4(E_1^0 - E_2^0 + W_{11} - W_{22})^2 + |W_{12}|^2},\\
\psi_2 = B(\varphi_{2p_0} + c_2\varphi_{2s}),\\
E_3 = E_3^0, \quad \psi_3 = \varphi_{2p_1}, \quad E_4 = E_4^0, \quad \psi_4 = \varphi_{2p_{-1}},
\end{gathered} \tag{14}$$

where

$$\varphi_{2p_0} = \pi^{-1/2}\beta^{5/2}e^{-\beta r}\,r\cos\theta, \quad \varphi_{2s} = [3\delta^5/\pi(\alpha^2+\delta^2-\alpha\delta)]^{1/2}\left(1-\frac{\alpha+\delta}{3}\right)e^{-\delta r},$$
$$\varphi_{2p_1} = \pi^{-1/2}\lambda^{5/2}e^{-\lambda r}\,r\sin\theta\sin\varphi, \quad \varphi_{2p_{-1}} = \pi^{-1/2}\lambda^{5/2}e^{-\lambda r}\,r\sin\theta\cos\varphi. \tag{15}$$

The values $E_1^0 = E_3^0 = E_4^0$ were determined by Pekar;[2] it is convenient to display them in the form

$$E_1^0 = E_3^0 = E_4^0 = -(\mu e^4/2\hbar^2\varepsilon^2)\,{}^1\!/_4\,[1+\varepsilon c f(v)]^2, \qquad f(v) = 1 - {}^1\!/_7\,(66v^3+84v^2+40v+7)/(1+v)^7, \tag{16}$$

$v = \alpha/\beta = \alpha/\lambda$ is determined from the equation

$$v = (3+\varepsilon c)/(1+\varepsilon c f(v)). \tag{17}$$

The values of E_2^0 and δ were specially calculated:

$$E_2^0 = -\frac{\mu e^4}{2\hbar^2\varepsilon^2}\,\frac{3\,[{}^1\!/_2\,(1+\varepsilon c)(s^2-2s+3)-\varepsilon c\Phi(s)]^2}{(s^2-s+1)(s^2-s+7)}, \qquad \Phi(s) = (53\,s^4+164\,s^3+193\,s^2+103\,s+21)/14\,(1+s)^6, \tag{18}$$

$s = \alpha/\delta$ is determined from the equation:

$$s = (3+\varepsilon c)(s^2-s+7)/6\,[{}^1\!/_2\,(s^2-2s+3)(1+\varepsilon c)-\varepsilon c\Phi(s)].$$

The frequency of the corresponding photo-transition is determined by the formula

$$\hbar\Omega_i = |E_0 - E_i|, \tag{19}$$

where E_0 is the Schrödinger term of the ground state of the F⁻ center

$$E_0 = J_0 + \frac{e^2}{\varepsilon R} - \frac{e^2 c}{2}\int \frac{\psi_0^2(1)\,\psi_0^2(2)}{r_{12}}\,d\tau_{12}. \tag{20}$$

The absorption coefficients are proportional to the squares of the moduli of the matrix elements

$$z_i = \int \psi_0(r)\,r\cos\gamma\,\psi_i(r)\,d\tau, \tag{21}$$

γ is the angle between the electric field intensity vector **E** and the radius vector of the electron **r**. Choosing for convenience the axis ac along the z axis, using the well-known relation

$$\cos\gamma = \cos\theta\cos\vartheta + \sin\theta\sin\vartheta\cos(\Phi-\varphi),$$

where θ and Φ are the spherical coordinates of the vector **E** and ϑ and φ of the vector **r**, and substituting Eqs. (5) and (14) in Eq. (21), it is possible to compute the values of the absorption coefficient of light for photo-transitions to the states Eq. (14). It is convenient to use the ratios of the absorption coefficients for the corresponding F⁻ and F absorption bands which can be written in the form

$$\begin{aligned} \xi_1 &= \tau_1^{F^-}/\tau^F = 2A^2\cos^2\theta\,(\Omega_1^{F^-}/\Omega^F)\,N_{F^-}/N_F,\\ \xi_2 &= \tau_2^{F^-}/\tau^F = 2B^2\cos^2\theta\,(\Omega_2^{F^-}/\Omega^F)\,N_{F^-}/N_F,\\ \xi_3 &= \tau_{3,4}^{F^-}/\tau^F = 2\sin^2\theta\,(\Omega_{3,4}^{F^-}/\Omega^F)\,N_{F^-}/N_F, \end{aligned} \tag{22}$$

if the irradiation is performed with polarized light; for natural light it is necessary to average over θ. In the expressions Eqs. (22), $\Omega_i^{F^-}$ and Ω^F denote the absorption frequencies of F⁻ and F centers respectively, N_{F^-} and N_F are the concentrations of F⁻ and F centers.

For the KCl crystal the calculations yield:

$$\begin{aligned} \hbar\Omega_1 &= 2.2 \text{ ev}, & c_1 &= 0.55, & \xi_1 &= 0.85\,N_{F^-}/N_F,\\ \hbar\Omega_2 &= 2.0 \text{ ev}, & c_2 &= 1.82, & \xi_2 &= 0.20\,N_{F^-}/N_F,\\ \hbar\Omega_3 &= \hbar\Omega_4 = 1.9 \text{ ev}, & & & \xi_{3,4} &= 0.95\,N_{F^-}/N_F. \end{aligned} \tag{23}$$

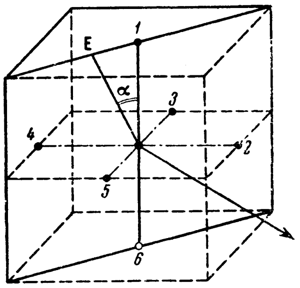
An estimate indicates that the total error of the calculation brought in through the use of an inexact wave function for the ground state of the F⁻ center Eq. (5) and by the neglect of a second approximation in perturbation theory is of the order of hundredths of an electron volt.

Thus, two absorption bands of rather large intensity correspond to the F⁻ bands, situated in the immediate vicinity of the F band. It should be pointed out that the frequency of light absorbed by F centers in KCl, calculated in the Franck-Condon approximation with the use of the functions Eqs. (5) and (15) turns out equal to 2.0 ev while the experimental value is 2.2 ev.

It is interesting to note that the lowest of the excited levels of the F^- center turns out to be a $2p\pi$ level and not a $2p\sigma$, as for example in the case of the H_2^+ ion or of the F_2^+ color center.

3. POLARIZED LUMINESCENCE OF F^- CENTERS

From the results of Sec. 2 it follows that the absorption and consequently also the emission of light by each individual F^- center is proportional to $\sin^2\theta$ for the long wavelength and $\cos^2\theta$ for the short wave F^- band. In a crystal, several possible orientations of F^- centers exist, for example, six in a crystal of the KCl type according to the number of nearest different charge neighbors of each ion. The calculation shows that this circumstance leads to a depencence of the degree of polarization of the emission brought about by polarized light on the direction of the electric field intensity vector **E**, and in some cases to a dependence of the total intensity of the emission on the polarization of the excited emission and to "spontaneous" polarization of emission. These dependences can be studied by means of the experiment performed by Feofilov[7] in the investigation of F_2 centers.



By way of example we consider one of the possible cases. From a crystal containing F^- centers let a platelet be cut having its face coincident with a 110 plane of the crystal. We shall excite F^- centers by light polarized in this plane; by rotating the crystal, one can vary the angle α between the vector **E** and the fiducial axis of the crystal (see figure). Further, the intensity of the emission in a direction perpendicular to the face of the crystal is measured as a function of the angle α and the degree of polarization of the emission is calculated.

Let us suppose for definiteness, that the excitation occurs in the long wave F^- band. Computation of the angle θ for each group of similarly orientated F^- centers permits the determination of the probability of absorption of light by each group of F^- proportional to $\sin^2\theta$:

$$W_1 = W_6 \sim \sin^2\alpha;\quad W_2 = W_3 = W_4 = W_5 \sim {}^1/_2(1+\cos^2\alpha). \tag{24}$$

Thus the number of F^- centers of each group excited by polarized light depends on α.

$$N_1 = N_6 = n\sin^2\alpha,\ N_2 = N_3 = N_4 = N_5 = (n/2)(1+\cos^2\alpha),\ n = \text{const}. \tag{25}$$

The probability of emission in a given direction for the i-th group of oscillators I_i^{em} is determined by means of integration of the functions Eqs. (24) over all possible directions of polarization of the emitted light; the total intensity of emission in a given direction is

$$J = \sum N_i I_i^{em} = c'\,[2\pi\sin^2\alpha + 3\pi(1+\cos^2\alpha)] = c\,(5+\cos^2\alpha) \tag{26}$$

and is in the given case a function of α.

The polarization of the emission is calculated according to the usual formula $p = \Sigma p_i I_i / \Sigma I_i$, where I_i is the intensity of light sent out in the direction of observation by each group of F^- centers and p_i are the partial polarizations determined according to $p_i = (J_{i\parallel} - J_{i\perp})/(J_{i\parallel} + J_{i\perp})$.

Below are presented the results of calculations for several cases; a crystal with the KCl type lattice is considered.

1. The face of the cut out platelet coincides with a 110 plane of the crystal.

(a) Excitation occurs in the long wave F^- absorption band. The emission occurs from this same excited level

$$J = c\,(5+\cos^2\alpha),\quad p = \frac{3\cos^2\alpha - 1}{\cos^2\alpha + 5}\cos 2\alpha. \tag{27}$$

It is easy to convince oneself of the existence of polarization of luminescence also for excitation with natural light ("spontaneous" polarization); calculation leads to the value

$$p_{sp} = \cos(2\alpha)/11. \tag{28}$$

(b) Excitation occurs in the short wave F^- absorption band; radiation proceeds from the same excited level

$$J = c\,(1+\cos^2\alpha),\qquad p = \frac{3\cos^2\alpha - 1}{1+\cos^2\alpha}\cos 2\alpha,\qquad p_{sp} = \frac{\cos 2\alpha}{3}. \tag{29}$$

(c) The excitation occurs in the short wave F^- absorption band; the emission proceeds from the lowest excited level (assuming that a non-radiative transition has taken place to the lowest excited level)

$$J = c(2+\sin^2\alpha), \quad p = \frac{1-3\cos^2\alpha}{2+\sin^2\alpha}\cos 2\alpha, \quad p_{\mathrm{sp}} = -\frac{\cos 2\alpha}{5}. \tag{30}$$

2. The face of the cut out platelet coincides with a 100 crystal plane.

$$\text{a) } J = 6c, \quad p = \frac{\cos^2 2\alpha}{3}, \quad p_{\mathrm{sp}} = 0, \qquad \text{b) } J = 2c, \quad p = \cos^2 2\alpha, \quad p_{\mathrm{sp}} = 0,$$
$$\text{c) } J = 2c, \quad p = -\cos^2 2\alpha, \quad p_{\mathrm{sp}} = 0. \tag{31}$$

For F_2 and F_2^+ centers according to references 5 and 7, cases (a) and (c) are realized.

The results Eqs. (27 — 31), generally speaking, differ from Feofilov's results[7] obtained with the hypothesis of absorption and emission of light by classical oscillators, the axes of which coincide with the axes of the F^- centers. Such a discrepancy is brought about by the unusual spacing of the excited levels of the F^- center as noted above.

4. COMPARISON OF THEORY WITH EXPERIMENT

The experimental investigations show that in the immediate neighborhood of the F absorption band under certain conditions additional bands arise situated on both the long and short wave sides of the F band. In particular, in Refs. 8 and 9 additional absorption bands were observed with a lower intensity F band. These former are masked upon increased intensity of absorption of light in the F band and apparently on this account they were not noticed by previous investigators. The frequencies of the absorption maxima of light in KCl for several of these bands are 1.76, 1.84, 1.94 and 2.03 ev, i.e., in rather good agreement with the results obtained during examination of the absorption of light by F^- centers. On the other hand, the absorption frequencies calculated in reference 5 for light in the F bands (1.91 and 2.22 ev for the intense F_2^+ band in KCl) are also very close to the experimental results of Yagi.[9]

One should note that the criterion of the macroscopic approximation used in the present work and in Refs. 3 — 5 in the alkali halide crystals for which the experimental data necessary for a comparison with theory is available, is not sufficiently well fulfilled for color centers.[2] Taking also into account the fact that in the range of frequencies in which the theory predicts the presence of the F_2^+ and F^- bands (1.8 — 2.3 ev in KCl) there is a whole series of very closely spaced bands, one must admit that a detailed comparison of experimental and theoretical results for the absorption frequency of light by the considered color centers is not possible in the given case.

The method considered in Sec. 3 of polarized luminescence of color centers, proposed by Feofilov[7] can be used for the precise identification of F^- centers.

I consider it my pleasant duty to express my appreciation to M. F. Deigen for valuable consultation.

---

[1] F. Seitz, Revs. Mod. Phys., 18, 384 (1946).

[2] S. I. Pekar, Исследования по электронной теории кристаллов (Investigations in the Electron Theory of Crystals), GITTL, 1951.

[3] M. F. Deigen, J. Exptl. Theoret. Phys. (U.S.S.R.) 21, 992 (1951); J. Exptl. Theoret. Phys. (U.S.S.R.) 24, 631 (1953).

[4] M. F. Deigen and V. L. Vinetskii, J. Exptl. Theoret. Phys. (U.S.S.R.) 32, 289 (1957), Soviet Phys. JETP 5, 226 (1957).

[5] V. L. Vinetskii and M. F. Deigen, Оптика и спектроскопия (Optics and Spectroscopy), (in press).

[6] Yu. E. Perlin, J. Exptl. Theoret. Phys. (U.S.S.R.) 20, 274 (1950).

[7] P. P. Feofilov, Dokl. Akad. Nauk SSSR 92, 545, 743 (1953); J. Exptl. Theoret. Phys. (U.S.S.R.) 26, 607 (1954).

[8] Uchida, Ueta and Nakai, J. Phys. Soc. Jap. 6, 107 (1951); Y. Uchida and H. Yagi, J. Phys. Soc. Jap. 7 109 (1952).

[9] H. Yagi, J. Phys. Soc. Jap. 11, 430, 723 (1956).

Translated by R. L. Eisner