On the Anderson Transition in Electronic Color Centers Systems in Alkali Halide Crystals

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An alkali halide crystal with a high concentration of F-centers is considered. If some of these F-centers are ionized into anion vacancies (α-centers) released electrons can be trapped by other F-centers to form F′-centers. It is shown that for each original concentration of F-centers there is a certain concentration of F′-centers for which the random potential fluctuations due to negatively charged F′-centers and positively charged α-centers have enough amplitude to create Anderson localization condition in the system of F-, F′- and α-centers.

Consider an alkali-halide crystal with a certain original concentration of F-centers N_F. Suppose next that one of these F-centers trapped an extra electron and formed a negatively charged F′-center. Since the potential fluctuations due to a random distribution of F-centers are very weak (F-centers are electrically neutral and their potentials fall off sharply) the formed state will be almost degenerate with any other state in which an extra electron is localized on another F-site. Physically this means that an extra electron of an F′-center is, in fact, delocalized and subjected to a spontaneous hopping-like activationless tunnel diffusion throughout the network of F-sites.

The usual process of the creation of F′-color centers consists of the (direct or via-the-excited-state) photoionization of a number of F-centers with the subsequent trapping of the released F-electrons by other F-centers [1, 2]. As a result a random distribution of negatively charged F′-centers and an equal number of compensating positively charged anion vacancies (α-centers) will be formed. Due to the long-ranged Coulomb fields of charged F′- and α-centers the random fluctuations of the crystalline potential will now have much greater amplitude than in the case of the presence of neutral F-centers only. The fluctuations of F′site's energies make the tunnel diffusion of extra electrons of F′-centers more difficult because electrons are no more able to conserve energy in the act of the tunnel hopping. The electron can only tunnel from one site to another if the time it spends on the second site is short enough that the uncertainty principle allows energy conservation to be violated to the necessary extent [3].

The question now arises as to whether these fluctuations are sufficient enough to produce the "true" quantum-mechanical localization of F′-centers in the sense of Anderson electronic localization (AEL). In the vicinity of the Anderson transition the very collective of extra electrons of F′-centers loses its ability to diffuse throughout the network of F-sites and this effect could, at least in principle, manifest itself in the discontinuities of some physical properties of the crystal (e. g. high frequency dielectric constant).

The amplitude of the potential fluctuations due to a random distribution of changed F′- and α-centers (which is of the order of the energy of the Coulomb interaction between two neighbouring charge centers) can be approximately found as [4, 5]

$$W \cong 2\, e_0^2 N_{F'}^{1/3}/\varkappa\,. \tag{1}$$

Here e_0 is an electron charge, $\varkappa$ is the dielectric constant of the material and the presence of factor 2 reflects the fact that there are *two* independent random distributions of oppositely charged defects with the same concentration (i. e. $N_{F'} = N_a$). Note, that one can also interpret W as the effective width of the F′-quasiband.

The condition of AEL can be formulated in the form [6]

$$W/V \gtrsim \eta\,, \tag{2}$$

where η is the constant of the order of a few units and V is the energy transfer integral between the nearest neighbor sites which were originally (i. e. "before" AEL) available for the electron jump. Here we identify V with the energy of g-u-splitting for a system of one F′-center shared between two equivalent F-sites. Applying the same approach as was used in the case of M′-center [7] one can obtain an expression for V in the delta-well potential model

$$V \cong \frac{2\,\gamma\, e_0^2\, a_0}{R}\, e^{-\gamma R}\,, \tag{3}$$

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where γ is the reciprocal radius of the wave function of an extra electron of an F′-center. Physically, the condition of AEL (Eq. (2)) means that the value of the transfer integral V is too small to ensure such quick jumps of the F′-electron between adjacent F-sites (which have their trapping energy spread randomly within the interval W) that the duration of its stay on each particular site (which is $\sim 1/V$) would be permitted by the uncertainty principle in the above mentioned sense.

Equation (3) is written in absolute units: $a_0 = 0.529$ Å is the Bohr's radius. For the distance R we take the mean separation between the sites potentially available for the localization of the extra electron of the F′-center, i. e.

$$R = N_F^{-1/3}. \tag{4}$$

Here N_F is the concentration of F-sites (and not of F′-centers!); we assume that $N_{F'} \ll N_F$, so that slight decrease of the order of $(N_F - N_{F'})/N_F$ in the number of the available F-sites can be ignored.

Combining Eqs. (1), (3) and (4) with the inequality (2) we obtain the following condition for the occurence of AEL in an F′-F-system

$$N_F^{1/3} \gtrsim \eta \varkappa(\gamma a_0) N_F^{1/3} \exp\{-\gamma N_F^{-1/3}\}. \tag{5}$$

To estimate the critical concentration of F′-centers we use the values (for KCl crystal): $\gamma = 0.28$ at units ($\gamma^{-1} = 1.89$ Å) [7] and $\varkappa = 4.68$ and take for η the value $\eta \cong 8$ as was obtained in [6] for the diamond-type site structure.

In Table 1 the critical values of $N_{F'}$ are calculated for $R = 4\,d_0$, $6\,d_0$ and $8\,d_0$ ($d_0 = 3.14$ Å is the lattice constant) which correspond to one F-center per 32, 108 or 256 anion sites respectively (it is not necessary to assume, however, that F-centers form an ordered superlattice with the period R).

Table 1. Critical concentration of F′-centers required for the occurence of Anderson localization for various mean distances R between neighboring F-centers in KCl crystal.

R	N_F cm^{-3}	$(N_{F'})_{crit}$ cm^{-3}
$4\,d_0 = 12.56$ Å	5.0×10^{20}	1.3×10^{15}
$6\,d_0 = 18.84$ Å	1.5×10^{20}	1.8×10^{10}
$8\,d_0 = 25.12$ Å	6.3×10^{19}	3.5×10^{5}

If for any particular N_F the concentration of F′-centers exceeds $(N_{F'})_{crit}$ then F′-centers will be localized in the sence of AEL. We are considering here an ideal case of $T = 0$ °K, so no temperature excitations are allowed. The only principle instability which will then still remain in the system of F′-, F- and α-centers will be due to the possibility of radiative-tunnel transitions [9] in F′ + α pairs. The probability of these transitions exponentially decreases with distance between neighboring F′- and α-centers, which is the order of $R_0 \sim N_{F'}^{-1/3}$. Since in our case $N_{F'} \ll N_F$ and consequently $R_0 \gg R$, the effect of radiative tunnel transitions on the established AEL in the system will be insignificant.

Except of the above mentioned possible discontinuity of the dielectric response (resembling the Mott's discontinuity of the conductivity at the mobility edge [3]) we do not speculate here on the other possible experimental verifications of AEL in F-F′-systems since the main purpose of this note was to demonstrate theoretically the principle possibility of this system to exhibit an Anderson transition.

[1] H. Rampacher, Z. Naturforsch. **20 A,** 350 (1965).
[2] D. Stocker, Z. Naturforsch. **23 A,** 1158 (1968).
[3] D. J. Thouless, J. Non-Crystall. Sol. **8–10,** 461 (1972).
[4] B. I. Shklovskii, Sov. Physics-Semiconductors **6,** 1053 (1973).
[5] A. A. Berezin, J. Phys. C: Sol. State Phys. **13,** L947 (1980).
[6] D. C. Licciardello and D. J. Thouless, J. Phys. C: Sol. State Phys. **11,** 925 (1978).
[7] A. A. Berezin, J. Phys. C: Sol. State Phys. **12,** L363 (1979).
[8] A. A. Berezin, Physics Letters **72 A,** 48 (1979).