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редакция журнала «Известия высших учебных заведений. Физика», тел. 53-33-35

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Quantum-Chemical Modeling of Radiation Defects Stabilization and Association in Alkali Haloid Crystals

A.T. Akilbekov, T.Sh. Salikbaeva, K.O. Kaliakparov, M.V. Zdorovets

Eurasian national university named after L.N. Gumilyov, Astana, Kazakhstan, tel. (3172)356783,

E-mail: mzdorovets@inbox.ru

Abstract – This paper is the initial point in the series of works on quantum-chemical modeling of the processes of association and stabilization of radiation defects depending on a halogen size in the face-centered alkali haloid crystals (AHC).

1. Introduction

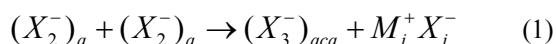
This paper presents a systematic quantum-chemical research, as well as comparative analysis of geometric and physical parameters of primary defects, namely H – centers and their associations in crystals of chlorides, bromides and potassium iodides. Also, the initial processes of interstitial halogen aggregation, which result in the creation of stable postradiational defects of a crystal lattice, are considered in the paper.

2. Modeling

Modeling has been performed with the help of MOPAC 7 quantum-chemical software package. A model cluster is represented as a cube of 6x6x6 ions. To facilitate the comparative analysis, the model clusters have the equal sizes for all three substances. The model crystal consists of 216 ions, 65 of which have the optimization of geometric parameters at the minimization of energy.

3. Results and discussion

It is known that the centers, which occupy two anionic and one cationic nodes of a lattice, form in AHC at $T \geq 80$ K. This fact proves the creation of the cationic Fraenkel defects. Therefore, the mechanism of cationic defect creation as a result of interaction of two H – centers was suggested, basing on the results of the experiment:

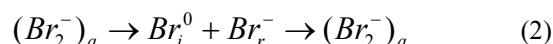


The geometric parameters of the H-center model have been calculated in the localized condition in KCl, KBr and KI crystals with the relaxation of the first coordination sphere taken into account.

The H – center is orientated along $\langle 110 \rangle$ crystallographic axis in KBr and KCl crystals; the energy of potential barrier of thermal delocalization is 0.07 and 0.22 eV accordingly; Br-Br bond length is 0.228 nm, Cl-Cl is 0.217 nm. Energetic parameters of delocalization which took place as a result of thermal annealing of H – centers, have also been calculated; they agree closely with the results of the experiments of H – centers annealing. According to the results of the modeling, the most energetically advantageous

mechanism of H – centers migration in a crystal is jumping diffusion along $\langle 110 \rangle$ crystallographic axis.

The process of H – center migration in a crystal can be described as the chain of chemical reactions:



The migration mechanism for both types of crystals is similar, and it is concluded in relay movement of a hole along the anionic sublattice.

Modeling in KI has shown that the center of the mass of iodine H – centre is greatly displaced to the center of the crystalline cell. In our opinion, this happens as a result of the ions of iodine having a greater ion radius than the ions of chlorine and bromine, and this corresponds to the results of modeling [1]. Also, the H – center of this crystal can have two types of orientation – either along $\langle 110 \rangle$ or $\langle 111 \rangle$ crystallographic axis, where the second case is 0.08 eV more energetically advantageous than the first one. The calculated value of the energy barrier of reorientation is equal to 0.05 eV. This could agree with the results of the experimental investigations [2], in which two picks (2.23 eV and 2.78 eV) were revealed in the absorption band of KI crystal, irradiated at 80 K. The results are presented in Table 1.

Table 1. Characteristics of the structure of AHC H – centers

crystal	bond length, nm	H-centre length, nm	orientation	energy of thermal delocalization, eV
KCl	0.3138	0.217	$\langle 110 \rangle$	0.22
KBr	0.3285	0.228	$\langle 110 \rangle$	0.07
KI	0.3525	0.258	$\langle 110 \rangle$	0.15
			$\langle 111 \rangle$	

According to the formula (1), $M_i^+ X_i^-$ interstitial dipoles must be created at the association of H-centers at $T \geq 80$ K. The performed quantum-chemical investigation of the location mode of a proper dipole in KCl, KBr, KI lattice has shown that $M_i^+ X_i^-$ dipole is localized in the lattice due to the formation of chemical bond with the ions of the nearest surrounding. Herewith, the dipole can exist in two

forms conditionally marked as N and Ψ forms. The N-form is organized due to the making of a chemical bond between the dipole ions and the two nearest node ions, where the node ions are displaced away from the dipole in $\langle 111 \rangle$ direction on (110) plane. The N-form is an intermediate stable form of dipole localization in a crystal lattice; it appears when dipole moves along the lattice. The calculations have shown that Ψ - form is generated due to the bond of dipole ions with four pairs of node ions, located in transverse, mutually perpendicular planes. The Ψ – form is the main configuration of dipole localization in a crystal lattice [3].

It has been calculated that a proper dipole can migrate in a lattice due to the relay transfer of anion and cation with small energetic consumptions (Table 2). The interstitial anion is transported along the anion sublattice, the cation is transferred along the cation sublattice; the dipole axis does not change its orientation.

Table 2. Geometric parameters and energy of the migration barrier of proper dipoles

crystal	dipole	dipole length, nm	energy of migration barrier, eV
KCl	$K_i^+ Cl_i^-$	0.2811	0.175
KBr	$K_i^+ Br_i^-$	0.2916	0.184
KI	$K_i^+ I_i^-$	0.3148	0.227

In crystals alloyed by cation impurities, the following dipoles have been considered: $Na_i^+ Cl_i^-$, $Li_i^+ Cl_i^-$ in KCl crystal, $Na_i^+ Br_i^-$, $Li_i^+ Br_i^-$ in KBr crystal and $Na_i^+ I_i^-$, $Li_i^+ I_i^-$ in KI crystal. Modeling of localization and migration of impurity interstitial dipoles has shown that these dipoles are localized in a crystal lattice in the same way as proper dipoles. The mechanism of the given dipole migration has turned out to be different from that of proper dipoles. At migration, the transfer of dipole is a combination of relay and diffusion mechanisms [4]. This means that the anion is transported along the anion sublattice, but the impurity cation diffuses into a nearby cell through a cube face. In the considered cases the potential

barrier of migration is several times greater than the migration barrier of proper dipoles (Table 3). According to the calculations, the existence of $Li_i^+ I_i^-$ dipole in KI crystal lattice is energetically not advantageous.

Comparing the data of energy of migration barrier, it can be concluded that the calculations have confirmed the experimental results, according to which the intensity of the formation of cation defects in the form of $(X_3^-)_{aca}$ – centers decreases in KCl→KBr→KI order.

Table 3. Geometric parameters and energy of the migration barrier of impurity dipoles

crystal	dipole	bond length of dipole, nm	energy of migration barrier, eV
KCl	$Na_i^+ Cl_i^-$	0.262	0.31
	$Li_i^+ Cl_i^-$	0.255	0.54
KBr	$Na_i^+ Br_i^-$	0.27	0.53
	$Li_i^+ Br_i^-$	0.269	0.8
KI	$Na_i^+ I_i^-$	0.299	0.45
	$Li_i^+ I_i^-$	-	-

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