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Experiment For Studying The Vacancy Migration In Divalent Doped Alkali Halide

Praveen Kumar Singh
Associate Professor- Physics S.G.N. Govt. P.G. College Muhammadabad Gohna Mau, (U.P.) India

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Abstract:An experiment has been proposed which helps in the study of the mechanism of vacancy migration in alkali halide lattice. In the presence of a static electric field, an alternating electric field applied in a perpendicular direction. The frequency of the alternating electric field is varied continuously and the required condition of maximum loss is detected experimentally. Proposed experiment has the potentiality to be used as a very sensitive and accurate tool for study of defect properties.

Key Words: experiment, proposed, study, mechanism, migration, lattice, presence, electric field.

Whenever a divalent impurity is introduced in an alkali halide matrix, a vacancy is created in the neighborhood of the impurity ion just for the sake of charge compensation. Impurity ion and the vacancy are oppositely charged and as such they result in the formation of an impurity vacancy (IV) dipole. With respect to the impurity ion, there are twelve nearest neighboring positions of cation vacancy (also of anion vacancy) in NaCl structure as shown in Fig. 1. Consequently, twelve equivalent orientations in the direction <110> are equally probable along which an IV dipole may lie. Out of the twelve equivalent orientations only three are inequivalent in the presence of an electric field. If the electric field E is applied along Z-axis, 4 orientations with the vacancy located at either of the sites 9 to 12 are in the unpreferred direction with the energy +eaE, 4 orientations with the vacancy located at either of the sites 5 to 8 are in the perpendicular direction with 0 energy and rest 4 Orientations with the vacancy located at either of sites 1 to 4 are in the preferred direction with the energy -eaE. Here e and a are electronic charge and anion-cation separation, respectively. The dipole in the preferred direction is oriented at an angle of 45° with respect to the direction of the static electric field. Once the orientation of the IV dipole under the influence of an external electric field is decided, the vacancy attached to the impurity ion may jump due to thermal agitation in an irregular way in all the four equivalent sites 1 to 4 with equal probabilities such as 1 ?2 ? 3 ?2?1 or 1 ?2 ? 3 ?2?3 ?4 ? 3 ?4?1 or in some other way. Activation energy for the orientation of IV dipole will not be obviously involved in such jumps. Also the applied electric field E will not influence the rate of such irregular jumps from one equivalent position to another equivalent one in between the sites 1 to 4 in XY plane. If the system is rapidly cooled down to a fairly low temperate , where the relaxation time becomes very -very large or practically infinite , the polarized dipoles are frozen-in in the system even in the absence of the applied static electric field. Thus, at such a low temperature vacancy attached to the frozen-in polarized dipole remains jumping in between the four equivalent site 1 to 4 even after switching off the electric field. The jump frequency of the vacancy from one equivalent site to its neighboring one will depend on temperate through the Boltzmann's factor. During such jumps it has to cross the saddle point for transition and it has to pass through the space available in between the two ions. The rate with which the vacancy jumps at the temperature T from one equivalent site to its neighboring one in between the sites 1 to 4 will be given by

$$?v= ?o\exp(-Ev/kT)$$

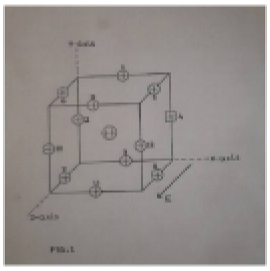

FIG.1

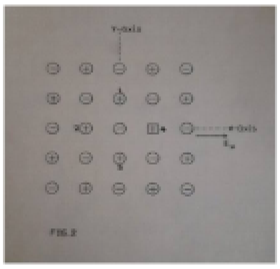

FIG.2

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were ?o is the effective vibrational frequency of the ions surrounding the vacancy, k the Boltzmann's constant and Ev the activation energy for the vacancy jump or the energy of migration of the vacancy. ?o is also known as the pre-exponential frequency or fundamental frequency which can be assumed to be equal to Einstein's lattice e frequency. It is obvious that the equivalent sites 1 to 4 will be separated from each other through a potential energy barrier of height Ev which an ion must surmount in order to pass to the adjacent vacancy. The vacancy will continue jumping in between the equivalent sites till the experimental temperature is not too low to restrict this jump. It would be justified to mention here that polarized dipoles are already frozen-in in the lattice as the activation energy for the orientation of dipole is higher than Ev .

The probability of finding the vacancy at any of the equivalent sites is statistically equal. Since the vacancies are jumping irregularly from one location site to its neighboring one, there will be no effective drift of the vacancy in any direction. If an additional electric field Ex is now applied along the X-axis as shown in Fig. 2, the vacancy starts jumping in such a way that it will ultimately occupy site 2. It should be mentioned just for the sake of reference that in divalent doped alkali halides, cation vacancy has higher mobility2 than anion vacancy as shown in Table 1.

The time required by the vacancy to have reached to the site 2 is expressed in terms of the relaxation time . To have an idea about the time dependence, let us consider for simplicity the situation corresponding to the location sites 1 and 2 which are separated by a potential energy barrier of height Ev as shown in Fig. 3. In the absence of the electric field Ev, the number of cation vacancies at the sites 1 and 2 will be the same and the vacancies will be jumping from one site to the other with the same frequency ?v. In the presence of the electric field Ev the potential energy curves will be modified as shown by dashed curve in Fig. 3. It is obvious from the figure that jumping from site 1 to 2 now requires less energy than that required to jump from site 2 to 1. Consequently, the number of cation vacancies at the site 2 will be more in comparison to that present at the site1.

Let us suppose that the applied electric field Ex is the alternating one and is changing in a time compared to , then the jumping cation vacancy on account of this time dependence cannot respond to the alternating electric field. If the polarity of the alternating electric field Ex reverses at the time when cation vacancy reaches at the site 2, the vacancy will be forced to jump either to the site 1 or to the site 3. Now, if the polarity of the alternating electric field reverses again at the instant when the vacancy just teaches either at the site 1or at the site 3, it will be activated by the alternating electric field to jump to the site 2. This process of to and fro mechanism of jump either in between the sites 1 and 2 of in between the sites 3 and 2 will continue provided

(/?) = ?v

where is the angular frequency of the alternating electric field applied along X axis. Such a situation will lead to the maximum value of the imaginary part of the permittivity or maximum loss which can be detected experimentally. It is proposed therefore that IV dipoles are polarized by applying a static electric field along z axis in a divalent doped alkali halide crystal, Now with the electric field still on, the system is rapidly cooled down to a fairly low temperature where the relaxation time is quite large or practically infinite. At such a low temperature, switching off the electric field keeps the polarized dipoles in frozen-in condition. An alternating electric field is applied either slang X axis or alone Y-axis. The frequency of the alternating electric field is varied continuously and required condition of maximum loss is detected experimentally. Such experiments recorded at different temperatures will result into the values of ?v at different temperatures. These values in conjugation with equation (1) give the values of ?o and Ev,

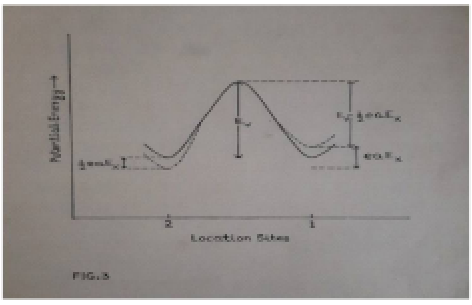

FIG.3

specifying the mechanism and characteristics of the vacancy migration in the lattice. If the temperature of investigation is kept low, the jump frequency ?v will be small suggesting that the maximum loss will appear at a lower frequency. For detecting the condition of maximum loss, such lower frequencies can be varied continuously without any experimental complications. Thus the proposed experiment has the potentiality to be used as a very sensitive and accurate tool for study vacancy migration in alkali halides.

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FIGURE CAPTIONS- Fig.1. Twelve nearest cation + neighbors to a divalent cation impurity ion ++ in NaCl structure. In the presence of a static electric field E along Z-axis, the cation vacancy + lies at any instant of time at the sitec4. Fig.2. Equivalent location sites 1 to 4 of the cation vacancy in the XY plane. Fig.3. Potential energy curves corresponding to the location sites 1 and 2 before (solids curve) and after (dashed curve) the application of the electric field Ex along X - axis.

Table. 1

Lattice	Enthalpy Of Migration (e.V.)	
	Cation vacancy	Anion vacancy
KCl	0.74	0.99
KBr	0.67	0.92
KI	0.63	1.29

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