expression in large parentheses becomes

$$S_n = \sum_{\lambda_1\lambda_2\lambda_3\cdots\lambda_{n-1};\lambda_i\neq\lambda_{i+1}} [\tau_\lambda(\vec{k}_t)G^{\lambda\lambda_1}(\vec{k}_t) \times\tau_{\lambda_1}(\vec{k}_t)\cdots G^{\lambda_{n-2}\lambda_{n-1}}(\vec{k}_t)\tau_{\lambda_{n-1}}(\vec{k}_t)]_{LL'}.$$

Summing over all values of n for the bracketed expressions in Eq. (20) leads to our definition of the matrix elements of the "layer" scattering matrix $||T_\lambda^{LL'}||$:

$$\Big(\tau_\lambda(\vec{k}_t) + \sum_{\lambda_1;\lambda_1\neq\lambda} \tau_\lambda(\vec{k}_t)G^{\lambda\lambda_1}(\vec{k}_t)\tau_{\lambda_1}(\vec{k}_t) + \sum_{\lambda_1,\lambda_2;\lambda_1\neq\lambda,\lambda_2\neq\lambda} \tau_\lambda(\vec{k}_t)G^{\lambda\lambda_1}(\vec{k}_t)\tau_{\lambda_1}(\vec{k}_t)G^{\lambda_1\lambda_2}(\vec{k}_t)\tau_{\lambda_2}(\vec{k}_t) + \cdots\Big)_{LL'} = T_\lambda^{LL'}(\vec{k}_t) \quad . \tag{28}$$

Equation (28) is just the power-series expansion of our desired coupled linear equations for the layer scattering matrices:

$$T_\lambda^{LL'}(\vec{k}_t) = \tau_\lambda^{LL'}(\vec{k}_t) + \sum_{\lambda';\lambda'\neq\lambda} \sum_{L_1L_2} \times\tau_\lambda^{LL_1}(\vec{k}_t)G_{L_1L_2}^{\lambda\lambda'}(\vec{k}_t)T_{\lambda'}^{L_2L'}(\vec{k}_t) \quad . \tag{29}$$

Insertion of Eq. (29) into Eq. (20) gives our final expression for the electron-solid scattering amplitude

$$R(\vec{k}_f,\vec{k}_i;E) = \sum_{LL'} Y_{L'}(\hat{k}_i)Y_L^*(\hat{k}_f)N_{\|}\sum_{\vec{g}}\delta(\vec{k}_i-\vec{k}_f+\vec{g}) \times\sum_\lambda e^{i(\vec{k}_i-\vec{k}_f)\cdot\vec{d}_\lambda}T_\lambda^{LL'}(\vec{k}_i) \quad , \tag{30}$$

in which the $\vec{g}$ are the reciprocal-lattice vectors of the Bravais net of the (identical) subplanes, and $N_{\|}$ is the number of cells per unit area.

Equations (25), (29), and (30) are identical to Eqs. (54), (55), and (2), respectively, in LD. Therefore, as noted earlier in the paper, the results of LD are correct, although the derivation given by LD of Eqs. (54) and (55) from Eqs. (32) and (48) is, perhaps, less transparent than the one given above.

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Off-Center Direction of Certain Atomic Impurities in Alkali Halide Matrices

G. K. Pandey and D. K. Shukla

Physics Department, Allahabad University, Allahabad, India

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The direction of the off-center displacement of certain atomic impurities in alkali halide matrices has been determined through calculations of certain barrier parameters. The controversial results for the RbCl: Ag^+ system and other systems like KCl: Li^+ and NaCl: Li^+ have been suitably discussed in the light of present calculations.

Recent experiments[1,2] have presented strong evidence for the off-centered position of certain atomic impurities in alkali halide matrices. For the RbCl: Ag^+ system, however, controversial results have been obtained by Kirby *et al.*[1] and Kapphan and Lüty.[2] The latter authors could explain their results on the basis of a ⟨111⟩ displacement direction, whereas the multiplet structure of the far-infrared absorption[1] ruled out such a configuration and presented evidence for a displacement in the ⟨110⟩ direction. We, in the present note, wish to present certain calculations of the barrier parameters, which will throw important light on this controversy concerning the displacement direction. For the sake of completeness, we also present calculations for the KCl: Li^+ and NaCl: Li^+ systems and

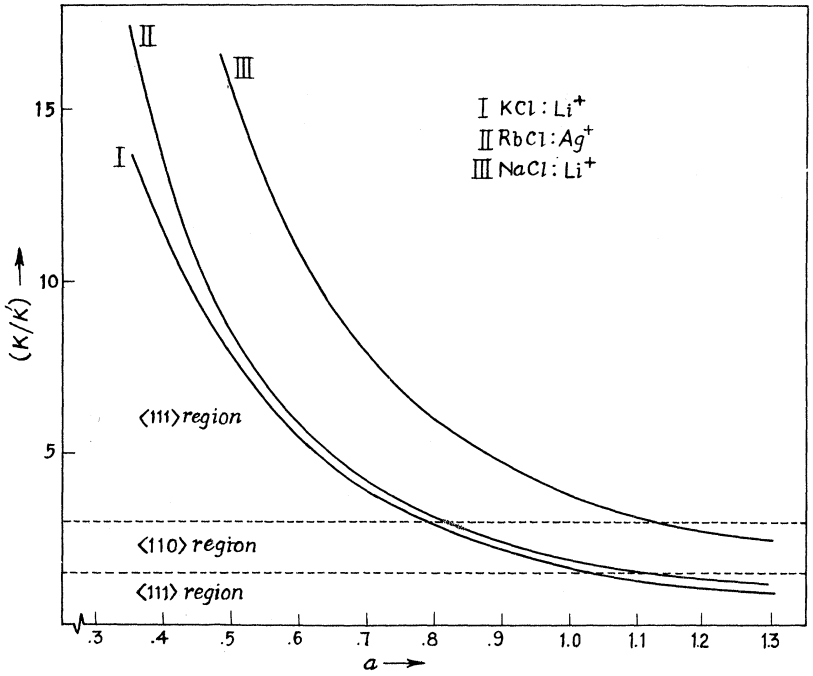

FIG. 1. Ratio K/K' as a function of off-center parameter a. Regions for ⟨111⟩ and ⟨110⟩ equilibrium orientations have been marked in accordance with the conclusion of Ref. 3.

determine the off-center directions in these cases as well.

It has been emphasized elsewhere[3] that the ⟨110⟩ orientation can be visualized only if one adds a V_6 term to the Devonshire octahedral potential. The Devonshire model considered only the first angle-dependent term V_4 in the expansion of the potential energy in an octahedral potential. It has been shown in Ref. 3 that if this expanded potential is written as

$$V(\theta,\phi)=K(\sin^4\theta\sin^2\phi\cos^2\phi+\sin^2\theta\cos^2\theta)+K'[\sin^6\theta(\sin^6\phi+\cos^6\phi)+\cos^6\theta]\,,$$

and if K/K' lies between 3.0 and 1.5, the minimum-energy configuration of the impurity will be along the ⟨110⟩ direction. Otherwise it will be in the ⟨111⟩ direction.

The coefficients K and K' can be obtained on the basis of two different specific models. One is the point-charge point-dipole model introduced by Lawless[4] and the other is the multipole-expansion model, recently developed by us.[5,6] For the cases of atomic impurities having no intrinsic dipole moment, both of the models give identical results. A simple calculation yields the following results for the parameters K and K':

$$K=\frac{C_HC_s}{R}\left\{\left[\frac{35}{2^2}\left(\frac{a}{R}\right)^4+\frac{3465}{2^5}\left(\frac{a}{R}\right)^8\right]_{\text{1st shell}}+\left[\frac{35}{2^3 3^4}\left(\frac{a}{R}\right)^4+\frac{3465}{2^6 3^6}\left(\frac{a}{R}\right)^8\right]_{\text{2nd shell}}+\text{similar terms for next shells}\right\}$$
$$+\frac{\alpha_HC_s^2+\alpha_sC_H^2}{R^4}\left\{\left[5.2^4\left(\frac{a}{R}\right)^4+105.2^4\left(\frac{a}{R}\right)^8\right]_{\text{1st shell}}+\text{similar terms for next shells}\right\},$$

$$K'=\frac{C_HC_s}{R}\left\{\left[\frac{231}{2^3}\left(\frac{a}{R}\right)^6\right]_{\text{1st shell}}+\left[\frac{231}{2^4 3^6}\left(\frac{a}{R}\right)^6\right]_{\text{2nd shell}}+\text{similar terms for next shells}\right\}$$
$$+\frac{\alpha_HC_s^2+\alpha_sC_H^2}{R^4}\left\{\left[7.2^7\left(\frac{a}{R}\right)^6\right]_{\text{1st shell}}+\text{similar terms for next shells}\right\}.$$

Here R is the lattice constant of the host crystal and a is the off-center displacement of impurity in the host matrix. α and C represent polarizability and charge, respectively, where the subscripts H and s stand for host-lattice ion and impurity ion, respectively.

In Fig. 1 we report the calculation of the ratio K/K' as a function of the off-center-position param-

eter a. In the same figure, we have marked the regions for the ⟨111⟩ and ⟨110⟩ orientations, based on the calculations of Mitra *et al.*[3] In our calculations we have considered different summations up to the fourth-neighboring shell of the impurity. For the RbCl: Ag^+ system, it can be seen that if the off-center position exceeds the value 0.82 Å, a ⟨110⟩ direction of displacement becomes more probable. The experimentally observed value for this parameter is 0.83 ± 0.08 Å,[1] establishing the fact, that probably this is an example of a borderline case. This can explain the reason of the controversy observed by the two authors. Our calculations of K/K' are for highly ordered crystal matrices. Dislocations and other imperfections near the impurity may stabilize a ⟨111⟩ position. Hence, the reason of the controversy may be attached to the use of improperly grown crystals and to the fact that this is an example of a borderline case for the orientation along ⟨111⟩ and ⟨110⟩ directions. For the KCl: Li^+, the figure shows that for values of a greater than 1.08 Å, a ⟨111⟩ off-centered position is plausible. The off-centered position observed experimentally is 1.2 Å,[5] confirming the ⟨111⟩ direction of displacement. This is in agreement with many other experimental results.[7,8] For the NaCl: Li^+, a ⟨110⟩ direction can be predicted only if a becomes greater than 1.12 Å. Such a high value of displacement in a NaCl matrix (lattice constant = 2.81 Å) is highly improbable. Hence in this system also a ⟨111⟩ direction of the off-center displacement is expected. This is in agreement with the results of Wilson *et al.*[9]

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Observation of Defect Annealing in Neutron-Irradiated Silicon by Space-Charge-Limited Current*

T. J. Magee,† A. M. Hermann, and R. J. Deck
Department of Physics, Tulane University, New Orleans, Louisiana 70118
(Received 1 October 1971)

Space-charge-limited current (SCLC) has been used to observe defect annealing in neutron-irradiated silicon. From the observation of the trap-filled-limit voltage a deep-trap concentration in the irradiated unannealed crystals is found to be at least 1.4×10^{12} cm^{-3}. Shallow traps are also observed. This deep-trap concentration decreases with anneal temperature up to 200 °C, above which SCLC can no longer be observed. There is evidence that at least some of this decrease is due to the conversion of the deep traps to shallow traps.

We report here observations of defect annealing in fast-neutron-irradiated silicon by the study of space-charge-limited current (SCLC). From the observation of trap-filled-limited voltages[1,2] (V_{TFL}) followed by trap-limited space-charge-limited currents,[2] we find evidence for at least two kinds of traps, deep and shallow, with a conversion of the former to the latter with increasing anneal temperature.

Single-crystal silicon wafers were obtained from Semi-Elements Co. and diced into small chips of cross-sectional area ≤ 0.35 cm^2. The current path was along the [111] direction in arsenic-doped and in phosphorus-doped crystals. Room-temperature resistivities prior to irradiation ranged from 4 to 12 Ω cm. Neutron irradiation was performed in the reactor at Wright-Patterson Air Force Base, Ohio, to a fluence of 10^{19} neutrons/cm^2. The irradiated samples were isothermally annealed for 20 min at each temperature. All current-voltage measurements were obtained on irradiated samples which were coated along the faces with a thin layer