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Influence of Ultrasound on Ionic Diffusion Process in Semiconductors

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It is well known that diffused ions are distributed over discrete energy levels and states of the continuous spectrum at a given temperature. This is usually a Boltzmann distribution. In the presence of an ultrasonic field, this is no longer true. In a sample where ion diffusion takes place, an anisotropy appears along the lines of propagation of the ultrasonic plane wave. The activation energy of the ion diffusion decreases in this direction by $\langle E \rangle$ (average value of energy transmission from the phonon gas to diffusing ions). The calculation of $\langle E \rangle$ was performed by Woodruff and Ehrenreich's methods /1/, which have been considered to be a completer form of the Boltzmann equation for the generalization of Akhieser's mechanism /2/. According to this mechanism the ultrasonic wave modulates the frequencies of all thermal phonons, changing their energy distribution.

It is convenient to analyse three systems: i) the interacting sound wave; ii) the dissipative system: the phonon gas, propagating sound wave; and iii) the thermostat.

The attenuation of sound waves is considered as a process of energy transmission from the wave to the phonon gas, which in its turn transmits some energy to the thermostat. As shown in /3/ it can be calculated either from the rate of transmission of energy from the sound wave to phonons, or its equivalent, i.e. the rate of energy transfer from the phonon gas to the thermostat.

If a system of diffused atoms is selected as a thermostat, then it will be natural to expect that the process of energy transmission to such a "thermostat" leads to a decrease of the ion lifetime in interstitial diffusion, i.e., to a decrease of the activation energy.

The diffusion coefficient will be presented as follows:

$$D = D_0 \exp \left\{ - \frac{Q_a - \langle E \rangle}{kT} \right\}, \quad (1)$$

where D_0 frequency factor, Q_a usual activation energy (without ultrasound effect), $\langle E \rangle$ the averaged value (with respect to time) of transmitted energy from the phonon gas to the thermostat. The ultrasound wave is assumed to be a travelling plane wave

$$\sigma = \sigma_0 \cos(\omega_s t - \vec{k} \cdot \vec{r});$$

here σ_0 amplitude of strain, caused by the ultrasonic wave and ω_s ultrasonic frequency.

Periodical changes are induced in the whole thermal phonon mode ensemble in a crystal, as a result of the propagation of such a wave. The distribution energy of thermal phonons becomes non-equilibrium. As being a dissipative system, the thermal phonon ensemble transmits energy to diffused ions by collisions. The Hamiltonian function for separate phonons in the point z (if the ultrasonic wave propagates along the z axis) at the moment t , taking into account an ultrasonic wave influence, will be /1/

$$H(\vec{q}, z, t) = H_0(\vec{q}) + H_1(\vec{q}, z, t) = \hbar \omega(\vec{q}, z, t), \quad (2)$$

where

$$H_0(\vec{q}) = \hbar \omega_0(\vec{q}),$$

$$H_1 = a(\vec{q}, \vec{k}, \sigma_0) H_0(\vec{q}) \exp \{i(\omega_s t - k_z z)\}.$$

Hence, the perturbation phonon frequency is

$$\omega(\vec{q}, z, t) = \omega_0(\vec{q}) (1 + a \exp \{i(\omega_s t - k_z z)\}), \quad (3)$$

where $\omega_0(\vec{q})$ frequency of the phonon mode in a non-deformed crystal by an ultrasonic wave, $a(\vec{q}, \vec{k}, \sigma_0)$ coefficient, the value of which is determined by elastic properties of the crystal.

The latter factor depends on the change of phonon mode frequencies under the effect of deformation. For describing the process of phonon collisions, by way of which the thermal phonon ensemble transmits the energy to the thermostat, we use the Boltzmann equation (for the one-dimensional case) where only first-order terms are preserved

$$\left(\frac{\partial N}{\partial t} \right)_{\text{coll}} = \frac{\partial N_1}{\partial t} + \frac{1}{\hbar} \left(\frac{\partial N_1}{\partial z} \frac{\partial H_0}{\partial q_z} - \frac{\partial N_0}{\partial q_z} \frac{\partial H_1}{\partial z} \right), \quad (4)$$

where $N(\vec{q}, z, t) = N_0(\omega_0) + N_1$ the perturbed distribution function, $N_0(\omega_0) = 1/(\exp(\hbar\omega_0/kT) - 1)$ the equilibrium distribution at temperature T .

According to [3], we have

$$-\left\langle \frac{\partial W}{\partial t} \right\rangle \equiv Q = - \sum_{q,j} \left\langle H \left(\frac{\partial N}{\partial t} \right)_{\text{coll}} \right\rangle, \quad (5)$$

where $-\langle \partial W / \partial t \rangle$ the average rate of phonon energy transmission to the "thermostat".

In (5) each mode is determined by a wave vector \vec{q} and polarization \vec{j} . For calculating $(\partial N / \partial t)_{\text{coll}}$ we use the relaxation time τ , specified by two scattering processes $1/\tau$, N processes where the wave vector is preserved and U processes that do not preserve it. A simple model is considered, where τ_N and τ_U are independent of \vec{q} and for which the frequencies have a simple Debye form:

$$\omega(\vec{q}, j) = v q;$$

here v is the constant average velocity of sound.

For the region $\omega_s \tau \ll 1$, in the case when $\tau_N / \tau_U \gg 1$ we have

$$Q = \alpha(\omega_s) J_s; \quad (6)$$

here J_s is the ultrasound wave intensity, $\alpha(\omega_s) = \kappa T \tau^2 \omega_s^2 / \rho v^5$ is the ultrasound attenuation coefficient, κ is the phonon thermal conductivity coefficient, γ is the Grüneisen constant, ρ is the crystal density.

Thus by collisions during the time t_s in a volume V , the thermal phonon assemble transmits the energy

$$\langle E \rangle = Q t_s V. \quad (7)$$

As it is seen from (7), the average phonon gas energy transmitted to diffused ions is determined mainly by the attenuation coefficient and the intensity of ultrasound. Fig. 1 shows the concentration variation (in arbitrary units) $C(z, t) = N(z, t)/N_0$ of diffused Li ions in p-Si along the depth z for different ultrasound frequencies ω_s .

This diffusion can be described by the equation

$$\frac{\partial N(z, t)}{\partial t} = D \frac{\partial^2 N(z, t)}{\partial z^2} \quad (8)$$

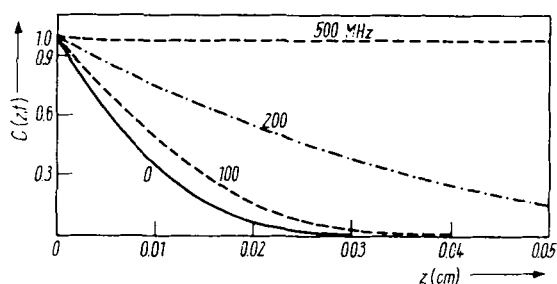


Fig. 1. Concentration distribution of diffused Li ions in p-Si for different ultrasound frequencies. $\tau_{av} = 4.15$ for Si, $T = 460$ K, diffusion time $t = 100$ h; $J_s = 10^8$ A/s cm²

with the initial concentration distribution $N(0, t) = N_0$, $N(z, 0) = 0$. In (8) the diffusion coefficient D is determined by relation (1). For an ultrasound frequency of the order of 500 MHz in expression (1)

$$\exp \left\{ - \frac{Q_a - \langle E \rangle}{kT} \right\} = 1, \quad D = D_0$$

and as it can be seen from Fig. 1, the concentration of diffused Li ions for this frequency practically remains unchanged along the depth of the p-Si sample.

We expect that the calculations given above will be useful in the compensation in lithium-drifted semiconductor detectors /4/.

References

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