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MODEL OF HOPPING BETWEEN DEEP CENTERS IN LOW TEMPERATURE GaAs*

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A model explaining hopping conductivity via EL2 deep centers in low temperature GaAs is presented. It is proposed that the wave function of the EL2 center consists of a localized part and of an external one. The model can describe such features as large wave function radius of hopping centers, changes of the conductivity during transition of EL2 to the metastable state and a high potential fluctuation amplitude.

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One of the most important features of the low temperature GaAs (LT GaAs) layers is unusually high content of arsenic (of the order of 1% more than gallium) causing high concentration of arsenic antisite defects (of the order 10^{20} cm^{-3}), high enough to create a deep defect band. It has been shown that in as grown LT GaAs layers hopping conductivity between arsenic antisite defects exists [1].

Hopping theory was developed for shallow centers. It takes into account that electron wave function has asymptotic behavior $\exp(-r/a_f)$ (a_f is called a wave function radius). Interaction of two neighbor centers and probability of electron transfer is thus proportional to an overlap of the wave functions. This assumption means that the transfer rate is proportional to $\exp(-\Delta r/a_f)$, where Δr is a distance between the centers. Moreover, in real crystal, there are fluctuations of local potential caused by existence of charged centers. Therefore, the energy $\Delta\varepsilon$ is needed for electron transfer between two centers with different potentials. Calculations made on the base of percolation theory give the equation for conductivity σ_3 [2]:

$$\sigma_3 = \sigma_{03}\exp\left(-\frac{\varepsilon_3}{k_B T}\right), \qquad \text{where} \qquad \sigma_{03} = \sigma_{003}\exp\left(-\frac{1.73}{a_f N^{1/3}}\right) \tag{1}$$

and where N is the concentration of hopping centers, ε_3 is an average energy difference between the two centers. In lower temperatures the dependence of conductivity versus temperature is characterized by Mott's law

$$\sigma = \sigma_{04}\exp\left[-(T_0/T)^{1/4}\right]. \tag{2}$$

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Transport characteristics of LT GaAs (Fig. 1) are in full agreement with these equations [2, 3], but some experimental facts about hopping conductivity in LT GaAs still remain to be explained:

1. Usually we treat the deep defect as an ion perturbed by a field of surrounding atoms of the crystal. In this approximation we obtain an electron wave function $\Psi_D(r)$ with the radius of about 1 Å. Instead, radius of 5–8 Å was reported [1, 3]. Moreover, recently scanning tunneling microscope (STM) pictures of arsenic antisite were obtained [4] showing that its wave function is much more extended than predicted from the deep level model.

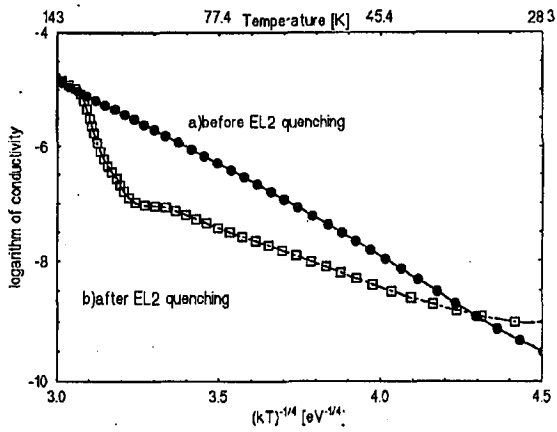

Fig. 1. Conductivity of LT GaAs plotted in the characteristic of hopping $T^{-1/4}$ scale (see Eq. (2)). (a) EL2 in the fundamental state, (b) EL2 in the metastable state.

2. It was observed that the excitation of EL2 to the metastable state causes great changes in hopping conductivity of the samples (see Fig. 1). It suggests that the changing of configuration switches off the center from hopping transport.

3. The energy ε_3 can reach 0.2 eV (in as grown material). The average difference of potential equals 0.2 eV and an average distance between centers of about 20 Å (see Fig. 2) suggest existence of an electric field $E = 10^6$ V/cm. Therefore high values of the energy and the electric field need also some explanation.

In the present approach, we took the Hamiltonian H_S containing not only the local potential of deep defect V_D but also a sum of the atomic potentials V_A of the crystal. We chose a wave function for the electron trapped at the deep defect in the form

$$\Psi(r) = \sqrt{1-\eta^2}\Psi_D(r) + \eta A(k) \sum_i e^{ikr_i}\Psi_A(r - r_i), \tag{3}$$

where the second term represents the Bloch-like function in LCAO approximation Ψ_B having an amplitude η. Resolving this problem, we obtain the expression

$$\eta^2 = (1 - \Delta H/\sqrt{\Delta H^2 + H_{BD}^2})/2, \tag{4}$$

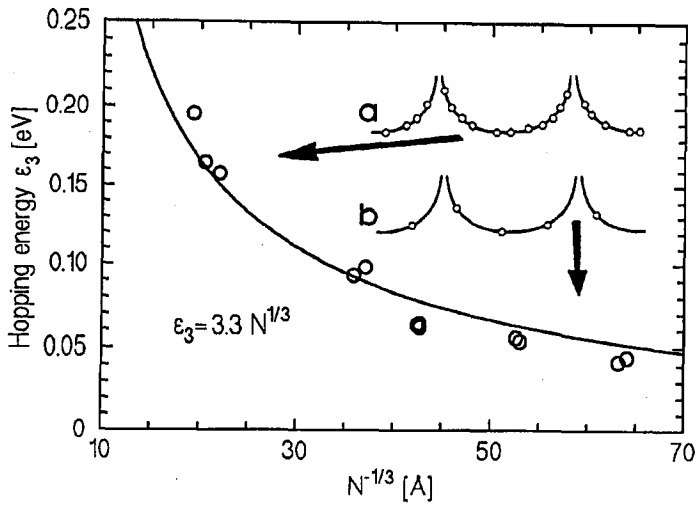

Fig. 2. The energy ε_3 versus average distance between EL2 centers $r_c \sim N^{-1/3}$: *a* — if r_c is small influence of acceptors is high, *b* — if r_c is big the potential fluctuations ($\approx \varepsilon_3$) are small. The curve represents $\varepsilon_3 = AN^{1/3}$ fit with $A = 3.3$ eV Å.

where $\Delta H = (\langle\Psi_B|H_S|\Psi_B\rangle - \langle\Psi_D|H_S|\Psi_D\rangle)/2$, $H_{BD} = \langle\Psi_B|H_S|\Psi_D\rangle$. If the interaction energy H_{BD} is equal to zero the amplitude η is also equal to zero. For the arsenic antisite Ψ_D is a function with symmetry $A_1(T_d)$ centered at gallium position, having radius of 1–2 Å. Therefore, H_{BD} will be reasonably high only for Ψ_A functions forming conduction band which are shifted to gallium places and have S symmetry. For these functions we get

$$k = \frac{\mathrm{i}}{\hbar}\sqrt{2m^*E}, \tag{5}$$

where E is approximately the energy level of the center counted from the minimum of conduction band.

If two centers taking part in hopping are at a distance few times longer than the radius of Ψ_D, the overlap between them will be proportional to $\eta^2\langle\Psi_B(r)|\Psi_B(r+\Delta r)\rangle$. This will affect Eqs. (1) and (2) by changing the preexponential factors σ_{003} and σ_{04}. They will be multiplied by η^2. In this situation the wave function radius a_f should be taken equal to $1/|k|$. For EL2, from Eq. (5) one gets $a_f = 8.7$ Å, which is in reasonable agreement with experiment.

In the fundamental state $\Psi_B(r)$ interacts with antibonding wave function of the EL2 electrons. The situation changes dramatically after the EL2 transfer to the metastable state. The As antisite is shifted by 1.4 Å to interstitial place [5] and antibonding electrons of the normal EL2 become nonbonding electrons of the metastable EL2. Localization of nonbonding state has to be much stronger than antibonding one. Therefore, interaction with Bloch function and its amplitude η should decrease. Indeed, we observed that when EL2 was in the metastable state the preexponential factor σ_{04} was about 100 times lower than in the fundamental state (see Fig. 1).

Since η is small, the amplitude of the wave function part localized on deep defect $(1-\eta^2)^{1/2}$ will be nearly equal to one. If this center is in a long range Coulomb potential of an acceptor we can treat it as a small object. Thus, the center placed at a distance r_a from the acceptor has the potential shifted by $\Delta\varepsilon = e^2/4\pi\varepsilon r_a$. The compensation ratio N_A/N_D in LT GaAs is about 0.01, therefore average distance from acceptor to the nearest donor is proportional to $N_D^{-1/3}$. It was found [6] that mainly the EL2 defects nearest to acceptors are ionized. Therefore we find that potential difference $\Delta\varepsilon$ should be proportional to $N_D^{1/3}$. Analysis of experimental results (Fig. 2) confirms this assumption.

In summary, the above-described model can be helpful in understanding of some peculiarities of hopping via deep defects. Especially high wave function radius a_f, hopping changes after EL2 transition to the metastable state and high potential fluctuation energy ε_3 are sufficiently explained.

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