25th International Conference on the Jahn-Teller Effect
Vibronic Coupling and Jahn-Teller Effects in Polyatomic System

Trigonal Jahn-Teller Complex V_{Ga}-Te_{As} in GaAs

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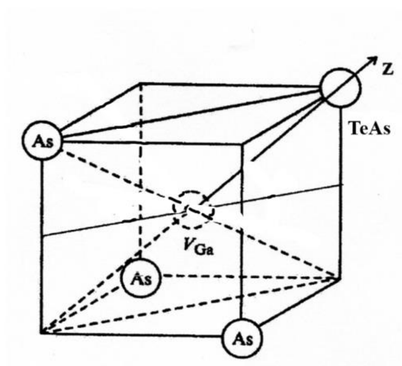
Deep levels in semiconductors

In semiconductors, there are two main types of impurities that give levels in the band gap: deep and shallow. The characteristic band gap is Eg~3 eV, if the ionization energy is $E_i=E_{sh}<<Eg$, then these are shallow impurities. If $E_i=E_d$ ~ Eg , then impurities giving deep levels. In any case, the characteristic size of the wave function of a localized charge carrier is $R_o \approx \sqrt{\frac{\hbar^2}{2mE_i}}$

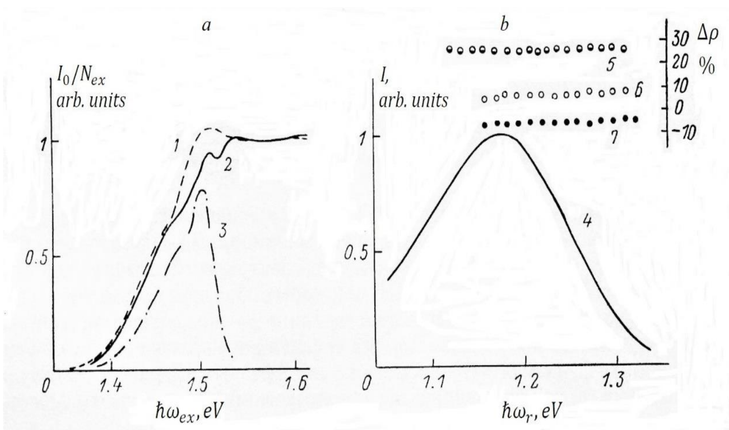
For shallow levels Ro>>a, for deep levels Ro~a, where a is the lattice constant. But there is an intermediate case $E_{sh}<E_i<E_d$ and then Ro~ (2-5)a.

In this case, the impurity atom + lattice atoms closest to it can be considered as a molecule and it can be assumed that the wave function of the charge carrier covers only the nearest neighbors. It is these impurities that will be considered in my report.

Vacancy complex in GaAs V_{Ga}-Te_{As}

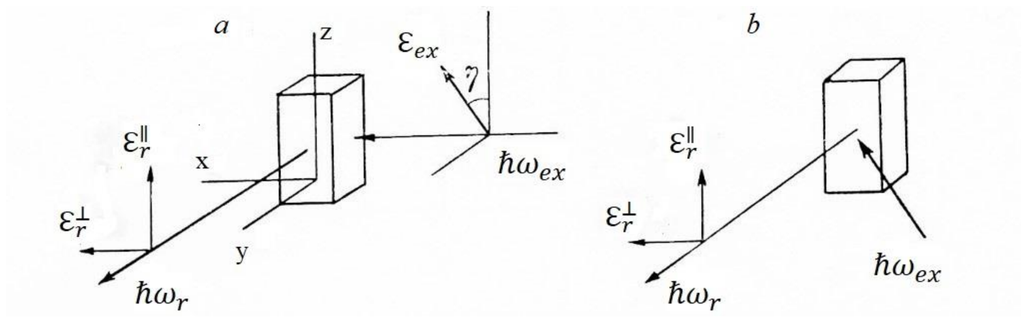


Photoluminescence spectrum of the $V_{Ga}Te_{As}$ complex



Photoluminescence of complexes $V_{Ga}Te_{As}$ n-GaAs:Te.
a–excitation spectrum photoluminescence at $\hbar\omega_r$≈1,2 eV;
b – photoluminescence spectrum and Δρ at $\hbar\omega_{ex}$= 1,43 eV.
T, K: 1, 3-7 – 77, 2 – 4,2.
1, 2 – scheme of the "reflection" experiment.
3-7 – orthogonal scheme of the experiment, the direction of propagation of the exciting (indicated first)) and the observed emitted light:
[011]-[100] – 5, [100]-[010] – 6, [110]-[10] – 7

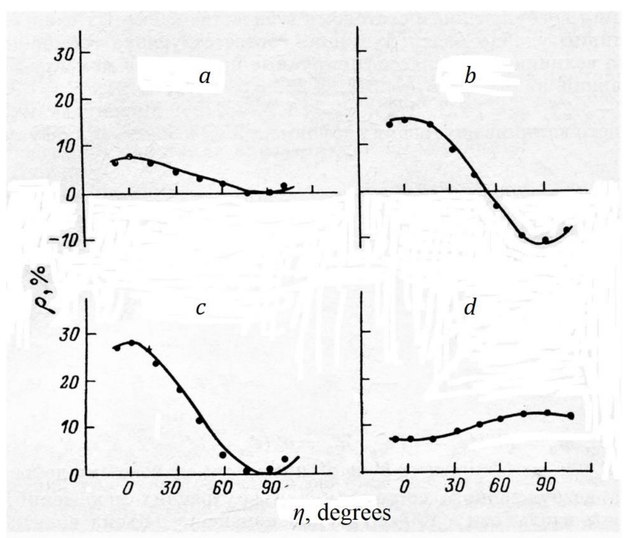
Experimental data



Resonance polarization spectroscopy
a – orthogonal scheme, b – “reflection” scheme.

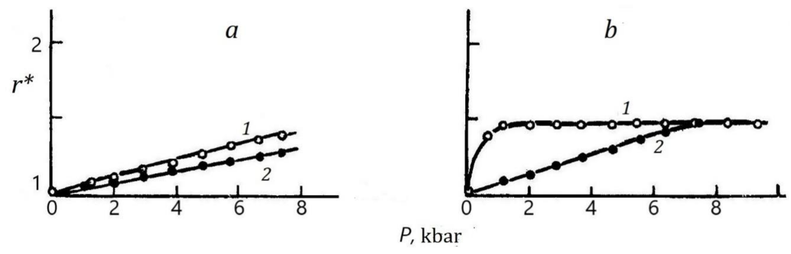
$\mathcal{E}_{ex}, \mathcal{E}_r^{\parallel}$ and $\mathcal{E}_r^{\perp}$ electrical vectors of the light wave of exciting and emitted light

Experimental data



Polarization diagrams of photoluminescence of complexes $V_{Ga}Te_{As}$ в n-GaAs:Te ($n_0 \approx \cdot 10^{17}$см$^{-3}$)
T = 77 K
$\hbar\omega_{ex}$ = 1,43 эВ
$\hbar\omega_r$ = 1,2 эВ
The orientation of the directions
of the excitatory (indicated first) and observed emitted light:
a – [100]-[010], *b* – [100]-[011],
c – [110]-[001], *d* – [110]-[110]

Demonstration of the anisotropy of the complex



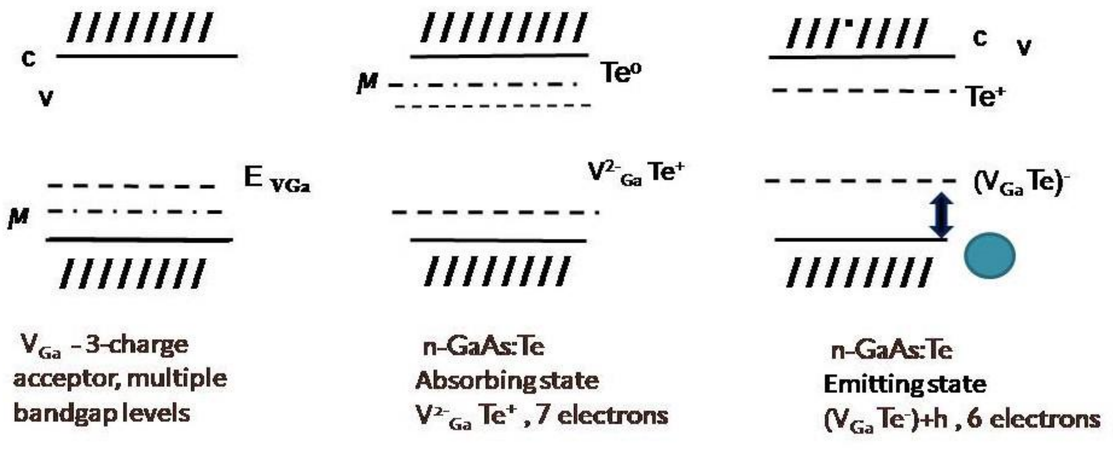
Experimental dependences of the polarization ratio of photoluminescence in the band with a maximum at the photon energy ~1,2 eV on the value of uniaxial pressure. Direction of pressure: *a* – [001],*b* – [111].
Excitation of photoluminescence by light from its own absorption band. T, K: 1 - 2, 2 - 77.

So, on the basis of experiments on resonant polarized spectroscopy and photoluminescence with interband excitation, it was established:

- In the emitting and absorbing states, the symmetry of the VGaTeAs complex is C2v
- At low temperatures, there is a reorientation of defects in the absorbing state
- The next task is to present a model that could explain these facts.

1. Gutkin,AA; Averkiev,NS Vacancy complex Ga-shallow donor in n-GaAs doping elements of VI group Te and S (Review). Semiconductors, 2022, number II,779 DOI: 10.21883/SC.2022.11.54956.9957

Model Charge states of a vacancy complex



The deepest level belongs to state of a_1 symmetry formed by the broken bond between the donor and the vacancy. The states with symmetry a_1 and e, formed by broken bonds of three As atoms surrounding the vacancy, and the level a1 is located closer to the conduction band than the level e . The strong interaction with the donor causes a significant distortion of the original wave functions of the vacancy .In this case, the symmetry of the wave function of the upper a_1 state does not change. Interaction of electrons in the a_1 and ewith non-totally symmetric phonons of E-type (Jahn-Teller pseudoeffect and Jahn-Teller effect) leads to further symmetry decreasing of the complex to monoclinic, to splitting of the electronic e-state, and a further change in the wave functions of electrons.

Model. Initial C_{3v} symmetry

In this case one can be assumed that the state a_1 with the deepest energy does not change under the influence of the electron-phonon interaction. Considering the interaction of the original trigonal complex with E-vibrations in a cubic lattice, it is convenient to introduce a new rectangular coordinate system in which the axis Z coincides with the volume diagonal of the cube containing the donor, and axis X lies in the plane of symmetry of the monoclinic center .The generalized coordinates of the E-vibrations associated with this system will be denoted by Q_x & Q_y . Then the Hamiltonian describing the donor influence and the interaction of one electron with E-vibrations in the basis of the original vacancy wave functions X, Y, Z has the form

$$\widehat{H} = \begin{pmatrix} -\Delta + F_2 Q_x & -F_2 Q_y & F_1 Q_x \\ -F_2 Q_y & -\Delta - F_2 Q_x & F_1 Q_y \\ F_1 Q_x & F_1 Q_y & 2\Delta \end{pmatrix}$$

For Q_x,Q_y= 0 λ_2 λ_3 = - Δ ,λ_1 = 2Δ

where 3Δ is the distance between the levels of the upper a_1- and e-states without electron-phonon interaction, F_1 and F_2 are constants describing the Jahn-Teller pseudoeffect and effect, respectively. Also note that in formula and the subsequent expressions following from it, it is impossible to assume Δ = 0, since in this case the symmetry of the complex is tetragonal, and the configuration of intrinsic vibrations of the atoms included in it is different. In the approximation of infinitely heavy nuclei, the wave functions ψi and energies of one-electron states λ_i (i = 1, 2, 3) are determined from the equation

$$H\psi_i = \lambda_i \psi_i$$

With Q_x , Q_y = 0, λ_2, λ_3 = −Δ, λ_1 =2Δ . At Q_x , Q_y are not equal to zero the expressions for λ_i become cumbersome, and further, for a qualitative consideration, we will use more simple expressions obtained under the condition that $F_1 \gg F_2$:

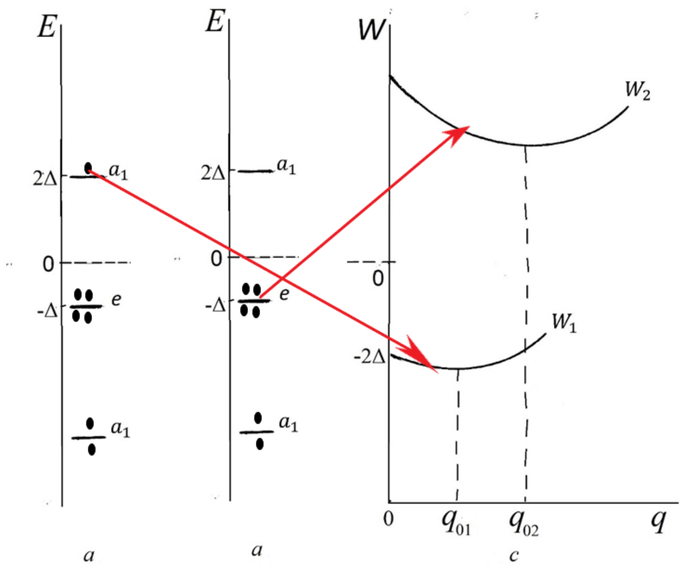
$$\lambda_1 = \frac{\Delta}{2} + \sqrt{\frac{9}{4}\Delta^2 + F_1^2 q^2} + \frac{F_1^2 F_2 q^3 \cos 3\beta}{2\left(\sqrt{\frac{9}{4}\Delta^2 + F_1^2 q^2} + \frac{3}{2}\Delta\right)\sqrt{\frac{9}{4}\Delta^2 + F_1^2 q^2}}$$

$$\lambda_2 = \frac{\Delta}{2} - \sqrt{\frac{9}{4}\Delta^2 + F_1^2 q^2} + \frac{F_1^2 F_2 q^3 \cos 3\beta}{2\left(\sqrt{\frac{9}{4}\Delta^2 + F_1^2 q^2} - \frac{3}{2}\Delta\right)\sqrt{\frac{9}{4}\Delta^2 + F_1^2 q^2}}$$

$$\lambda_3 = -\Delta - F_2 q \cos 3\beta,$$

where the designations Q_x = q cos β, Q_y = q sin β are introduced, and the angle β is measured in the plane XY from the axis X.

Model Charge states of a vacancy complex



Multi-electron scheme of levels in the absorbing and emitting state

W_1 - absorbing state

W_2 - emitting state

In the absorbing state the vacancy complex binds 7 electrons, two of which are at the deepest level, their energy makes a constant contribution to the energy of both absorbing and emitting states, and will not be taken into account. The remaining states, in which 5 electrons are located, change under the influence of JTE, and this must be taken into account when calculating the adiabatic potential of the center. Since $\lambda_1 + \lambda_2 + \lambda_3 = 0$, the total energy of these 5 electrons, neglecting the interaction between them compared to the influence of the donor and JTE , can be equal to $-\lambda_1$, $-\lambda_2$ or $-\lambda_3$. The minimum value of the total energy will be equal to $-\lambda_1$, i.e., under equilibrium conditions at low temperatures, there is one electron in the weakest bound state λ_1. To determine the equilibrium configuration of the complex in the absorbing state, it is necessary to determine the position of the minimum of the adiabatic potential W_1, which is equal to the sum of the total electron energy of 5 localized electrons and the energy of elastic vibrations

$W_1 = -\lambda_1 + K/2\ q^2$

where $K/2\ q^2$ is the elastic energy of E-vibrations of atoms, K is the elasticity coefficient. At $F_2 = 0$ W_1 is independent of β and is an annular trough with radius q_{01}. At $0 < |F_2| \ll F_1$, 3 minima of the adiabatic potential appear on this trough, which correspond to β = 0, 120 and 240◦ at F2 > 0.

In the emitting state 6 electrons are bound to the complex, and therefore only 4 electrons are localized in the considered upper states, and the fifth electron is in the conduction band. The minimum total electron energy of 4 electrons will be equal to $-2\lambda_1 + Ec$, where Ec is the electron energy in the c-band. In this case, the electronic state with energy λ_1 under equilibrium conditions at low temperatures is completely empty. In the emitting state, the adiabatic potential of the system complex + 5 electrons is

$W_2 = -2\lambda_1 + K/2\ q^2 + E_c$.

Since the electron in the conduction band does not interact with E-vibrations, Ec does not depend on q, and the form W_2 in the space of generalized coordinates of E-vibrations differs from W_1 only by the coefficient 2 before λ_1. As can be seen from equations for λ_i ,this is equivalent to replacing F_1, F_2 and Δ by $2F_1$, $2F_2$ and 2Δ, respectively. Thus, the efficiency of the JTE depends on the number of electrons localized on the complex, and in the emitting state the JTE is stronger than in the absorbing state. Accounting for this circumstance is a new result in the study of complex defects in semiconductors

Conclusion

The existence of an anisotropic trigonal Jahn-Teller defect in a cubic crystal is demonstrated. Such defects are V_{Ga}-TeAs and V_{Ga}-S_{As} vacancy complexes in GaAs.

The presented model of the center makes it possible to explain the entire set of experimental data. According to the model, the barriers between equivalent states are higher in the emitting state, so that the reorientation occurs in the absorbing state, in which the height of the barriers is several meV. Due to the different efficiency of JTE in different charge states, the optical dipoles in them are oriented differently.

Thank you for your attention