Temperature dependence of the lineshape of the $1s \rightarrow 2p_0$ photothermal ionization of donors in GaAs

S. D Baranovskiĭ, B. L. Gel'mont, V. G. Golubev, V. I. Ivanov-Omskiĭ, and A. V. Osutin

A. F. Ioffe Physicotechnical Institute, Academy of Sciences of the USSR, Leningrad

(Submitted 23 September 1987)
Pis'ma Zh. Eksp. Teor. Fiz. **46**, No. 10, 405–407 (25 November 1987)

A change has been observed in the lineshape of the $1s \rightarrow 2p_0$ photoexcitation of donors in GaAs which results from a transition from a correlated to a totally random distribution of electrons at impurities as the temperature is raised. A comparison of the experimental results with the results of a numerical simulation reveals the compensation and concentration of the impurities in the ultrapure GaAs.

Photoelectric magnetospectroscopy is the most sensitive and most precise method of analyzing the chemical composition of impurities in ultrapure semiconductors. The qualitative impurity composition is found from the positions of the lines in their photoexcitation spectra in a magnetic field. The high sensitivity of the method makes it possible to record photoexcitation spectra at impurity concentrations as low as[1] $\sim 10^5$ cm^{-3}. In the present letter we show that by comparing the temperature dependence of the lineshape of the $1s \rightarrow 2p_0$ photoexcitation of shallow donors with the results of a numerical simulation with and without consideration of correlations in the distribution of electrons among impurities one can determine the compensation and concentration of impurities in ultrapure GaAs. This capability extends the possibilities of photoelectric magnetospectroscopy.

Photoexcitation spectra are recorded by the procedure described in Ref. 2. We

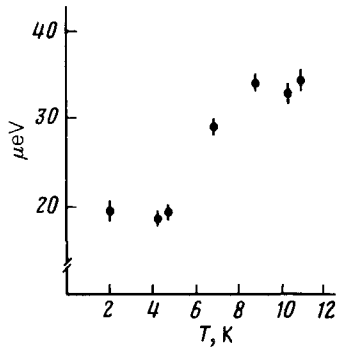

FIG. 1. Experimental temperature dependence of the half-width of the line corresponding to the $1s \rightarrow 2p_0$ photoexcitation of shallow donors in a GaAs sample ($\hbar\omega = 6.24$ meV, $H \approx 48$ kOe).

studied especially pure epitaxial layers of n-GaAs with a donor concentration $N_D \lesssim 10^{14}$ cm^{-3}, in whose photoexcitation spectra the line of donors of differing chemical nature can be clearly resolved.[3]

The temperature dependence of the half-width of the $1s \rightarrow 2p_0$ line at half-maximum has some structural features: At $T \leqslant 4$ K, the half-width is at a minimum and is approximately constant. As T is increased, this half-width increases, and it again reaches a constant value at $T \gtrsim 9$ K (Fig. 1).

In order to explain the observed temperature dependence, we need to consider the reasons for the broadening of the photoexcitation lines of impurities in GaAs. The primary reason for the broadening is the effect of the electric fields of the charged donors and acceptors. The lineshape near the maximum and at the half-maximum points is determined by the quadratic Stark effect and by the interaction of the quadrupole moments of the impurities with electric field gradients.[4]

In the especially pure and homogeneous layers of GaAs which we studied, the shape of the nonoverlapping $1s \rightarrow 2p_0$ lines in the spectra corresponding to chemically different donors is approximately symmetric. The quadratic Stark effect, which causes an asymmetric line broadening, is thus of minor importance in comparison with the quadrupole effect.[4] In this case the lineshape is described by the distribution function of the electric field gradients ($\epsilon_{zz} = \partial E_z / \partial z$) at neutral donors, where E_z is the component of the electric field along the magnetic field direction. At low temperatures, $T \ll e^2 N_D^{1/3} / k_B \kappa$ (e is the electron charge, κ is the permittivity of the material, and k_B is the Boltzmann constant), this distribution function is determined by a correlation in the arrangement of neutral and charged impurities due to the electron-electron interaction.[4] At high temperatures, $T \gg e^2 N_D^{1/3} / k_B \kappa$, the distribution of electrons among donors is approximately random.

The fact that there are two regions with a constant line half-width in the temperature dependence is evidence that the distribution of electrons among impurities changes from a correlated distribution to a random distribution in this temperature interval in GaAs. An estimate of the temperature of the transition from the correlated distribution to the completely random distribution, $e^2 N_D^{1/3} / k_B \kappa \sim 6$ K for $N_D \sim 10^{14}$ cm^{-3}, agrees with the abrupt changes seen experimentally in the linewidths.

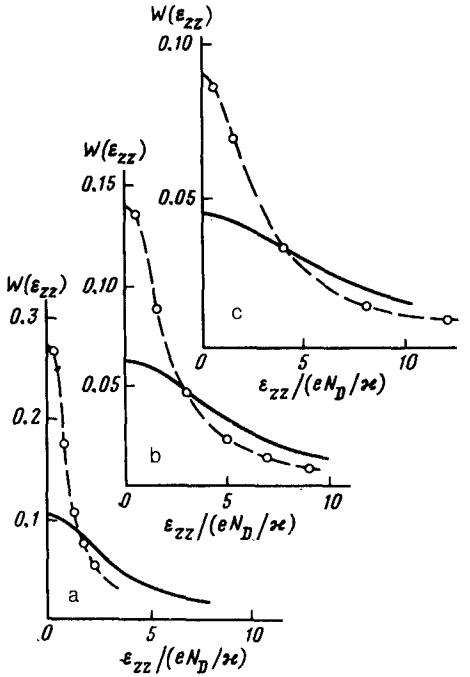

FIG. 2. Distribution function of the field gradient (the theoretical shape of the spectral line). The degree of compensation is a—$K = 0.3$; b—$K = 0.5$; c—$K = 0.7$. Solid lines—Results of Ref. 5;—points results of numerical simulation (the dashed lines are drawn to assist the eye).

To analyze the behavior of the linewidth as a function of the temperature, we need to calculate the distribution function of the field gradients for these two cases. For a random distribution of electrons among donors, this calculation has been carried out analytically by Larsen[5] and confirmed by a numerical Monte Carlo simulation. At low temperatures, where the filling of donors by electrons is determined by an electron-electron interaction, we carried out a Monte Carlo numerical simulation of the system. The simulation algorithm was similar to that used in Ref. 6. We also carried out analytic calculations based on the dipole model of Ref. 7, according to which the linewidth is proportional to $N_D \cdot K^{4/3}$. The results of the analytic calculations agree well with the results of the simulation. These results will be published in a more-detailed paper; here we are reporting only the results of the simulation.

Figure 2 shows the results of a calculation which applies to the case $T \ll e^2 N_D^{1/3}/k_B \kappa$, along with the data of Larsen,[5] which should be applied to the case $T \gg e^2 N_D^{1/3}/k_B \kappa$. We considered compensation values $K = 0.3$, 0.5, and 0.7. The switch from one type of electron distribution among impurities to the other results in a change in the linewidth, with a magnitude which depends on the compensation. The broadening increases with decreasing compensation.

In summary, a comparison of the linewidths for two distributions reveals the degree of compensation. If the compensation is known, a comparison of the experimental lineshape with the calculated lineshape can reveal the impurity concentration in a semiconductor.

[1]Sh. M. Kogan and T. M. Lifshits, Phys. Status Solidi **a39**, 11 (1977).
[2]V. G. Golubev, V. I. Ivanov-Omskiĭ, I. G. Minervin, A. V. Osutin, and D. G. Polyakov, Zh. Eksp. Teor. Fiz. **88**, 2052 (1985) [Sov. Phys. JETP **88**, 1214 (1985)].
[3]V. G. Golubev, Yu. V. Zhilyaev, V. I. Ivanov-Omskiĭ, G. R. Markaryan, A. V. Osutin, and V. E. Chelnokov, Fiz. Tekh. Poluprovodn. **21**, 1771 (1987) [Sov. Phys. Semicond. **21**, 1074 (1987)].
[4]Sh. M. Kogan and Nguyen Van Luen, Fiz. Tekh. Poluprovodn. **15**, 44 (1981) [Sov. Phys. Semicond. **15**, 26 (1981)].
[5]D. M. Larsen, Phys. Rev. B **8**, 535 (1973).
[6]S. D. Baranovskiĭ and A. A. Uzakov, Fiz. Tekh. Poluprovodn. **16**, 1606 (1982) [Sov. Phys. Semicond. **16**, 1026 (1982)].
[7]Sh. M. Kogan, Nguyen Van Luen, and B. I. Shklovskiĭ, Zh. Eksp. Teor. Fiz. **78**, 1933 (1980) [Sov. Phys. JETP **51**, 971 (1980)].

Translated by Dave Parsons