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IRON ADMINISTRATION IN GALLIUM ARSENIDE

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ABSTRACT

Based on the data obtained by nuclear gamma-resonance spectroscopy, it is concluded that the state of impurity atoms depends both on the type of conductivity and on whether these atoms are in the surface layer or in the bulk of semiconductors.

KEYWORDS: *Iron, Nuclear Gamma-Resonance Spectroscopy, Impurity Atoms, Surface Layer, Bulk of Semiconductors.*

INTRODUCTION

A number of works are devoted to the study of the properties of semiconductor compounds doped with iron. It has been shown, in particular, that the introduction of iron into GaAs leads to the appearance in the forbidden band of two deep-lying levels $E_0 + 0.37$ and $E_v + 0.52$ eV; however, until now it has not been clarified to which the indicated levels correspond to isolated iron atoms or the same complexes of the "impurity-impurity" type. It should also be noted that the concentration distribution of iron in GaAs after diffusion is characterized by two regions - near-surface and bulk.

MATERIALS AND METHODS

The complex concentration distribution, apparently, is caused by the different state of the impurity in the surface and bulk regions of the crystal. Since the parameters of the NGR spectra depend on the electronic structure and symmetry of the arrangement of impurity atoms in the crystal, it was of interest to study the state of iron atoms in GaAs by the Mössbauer method. The use of the emission version of spectroscopy made it possible to obtain information on impurity atoms both in the bulk of the sample and in its near-surface layer.

1. EXPERIMENTAL TECHNIQUE

As a starting material, we used p and n-type GaAs samples doped during growth with zinc ($p = 1.6 \cdot 10^{18} \text{ cm}^{-3}$) and tellurium ($n = 1.6 \cdot 10^{18} \text{ cm}^{-3}$). Samples in the form of plates were cut from single-crystal ingots oriented in the $\langle 111 \rangle$ direction.

The solubility of iron in GaAs is low ($\sim 10^{17} \text{ at-cm}^{-3}$ at 1050° C [4]), and therefore the emission version of spectroscopy was used to record the Mössbauer spectra - the ^{57}Co isotope was introduced into the samples under study, after the decay of which the Mössbauer level ^{57}mFe . Obviously, the information of emission Mössbauer spectroscopy refers to cobalt, when we mean the location of atoms in the lattice, the possibility of its complexation with lattice defects; and at the same time, this information refers to iron when it comes to the charge state of impurity atoms. In our experiments, ^{57}Co was electrolytically deposited on the surface of the samples, which were then subjected to diffusion annealing in evacuated quartz ampoules at 1050° C for 25 h. To reduce the evaporation of arsenic from gallium arsenide, a GaAs powder was placed in the ampoules, providing an equilibrium value of vapor pressure arsenic over the sample due to its evaporation from the powder. NGR spectra were recorded on an electrodynamic setup at 295° K with an absorber $\text{K4Fe (CN) } 6 \cdot 3\text{H}_2\text{O}$. The spectra were recorded twice - before and after removal of the surface layer ($\sim 150 \mu\text{m}$ thick).

Charge state and symmetry of the local environment of iron (cobalt) atoms in the near-surface layer of GaAs. The near-surface region is characterized by rather high concentrations of both impurity cobalt atoms and point defects (vacancies), and therefore in this region of the crystal there is a high probability of the formation of various kinds of associates with point lattice defects by impurity atoms.

Indeed, the observed broadening of the NGR spectra $\Gamma \wedge ^{57}\text{m Fe}$ in n-type samples indicates that iron (cobalt) is in a complex with vacancies. The value of the isomeric shift corresponds to the electronic configuration of iron, close to $3d^5$.

Since in n-type GaAs an isolated iron atom is ionized and has the $3d^5$ electronic configuration (see above), the observed $3d^5$ state of iron in the surface layer can be explained by the fact that isolated Fe ($3d^6$) atoms form a complex with a vacancy of the type $F \wedge (3) \text{ Ga } (3d^5) - V$. As a result, an electric field gradient (EFG) arises on the $^{57}\text{m Fe}$ nuclei, which can be calculated by the formula

$$\Delta E_Q = \frac{1}{2} eQ(1 - \gamma) \sum \left(\frac{3 \cos^2 \theta_i - 1}{r_i^3} \right) e_i^*$$

Where γ is the Sternheimer coefficient, r_i is the distance to the i -ion with charge e_i^* , θ_i is the angle between the principal axis of the EFG tensor and the direction r_i . Using this formula, the relative values of the quadrupole splitting of the NGR spectra of ^{57}mFe in various A3B5 compounds were calculated. It turned out that the calculated and experimental values of ΔE_Q [11] are in good agreement (Fig. 2). In p-type samples, the situation changes somewhat. Although the "iron-vacancy" associates remain, the impurity center is no longer ionized. As in the case of iron atoms in the GaAs volume, holes populate the $3d$ -shell of iron and thereby increase the electron density on ^{57}Fe nuclei.

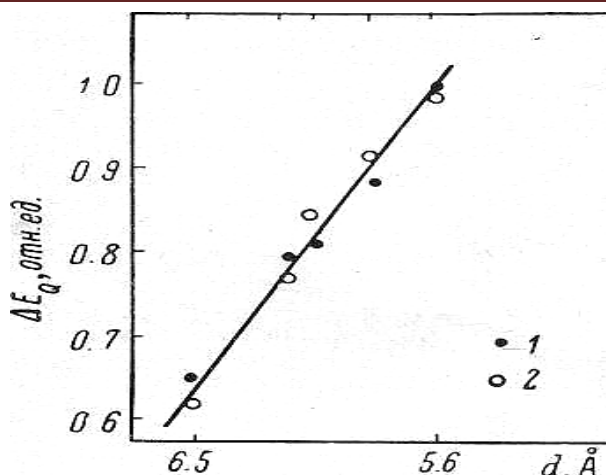


Fig. 2. Experimental (1) and theoretical (2) values of the quadrupole splitting of the NGR spectra of ^{87}Fe in compounds A_3B_5 . As a result, the quadrupole splitting of the NGR spectra should increase sharply, which is observed experimentally.

CONCLUSION

Thus, on the basis of the data obtained, it can be concluded that in the bulk of GaAs, impurity iron atoms are in a cubic environment and they can be regarded as isolated and the levels of iron found in [1, 2] can be attributed to these atoms. In the near-surface layer, iron atoms form complexes with vacancies and it can be assumed that other levels should correspond to such complexes (for example, in [3] such levels were detected by IR spectroscopy for iron atoms in the near-surface layer (GaAs)). Both for iron atoms in the bulk of the sample and for near-surface atoms, a charge exchange process is observed depending on the position of the Fermi level. Charge exchange affects the magnitude of the isomeric shift of the NGR spectra, i.e., the charge exchange changes the electron density on ^{57}Fe nuclei due to a change in the population of the 3d shell.

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