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Study of the Charging State of Impurity Iron Atoms in Gallium Arsenide

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ABSTRACT: The state of iron impurity atoms in GaAs depends both on the type of conductivity of the samples and on whether these atoms are in the surface layer or in the bulk of the sample.

KEYWORDS: Impurity, type of conductivity, spectrum, sample, quadruple doublet, concentration, charge exchange, isolated atom, and vacancy, complex.

I. INTRODUCTION

A number of works [1–8] are devoted to the study of the properties of gallium arsenide doped with iron. It was shown, in particular, that the introduction of iron in GaAs leads to the formation of two deep-lying levels of $E_v + 0.37$ and $E_v + 0.52$ eV in the band gap, however, it has not yet been clarified whether these levels correspond to isolated iron atoms or complexes of the << impurity type - admixture >>. It should also be noted that the concentration distribution of iron in GaAs after diffusion is characterized by two sections — near surface and bulk [9]. The complex concentration distribution is apparently caused by a 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 Mossbauer method. The use of the emission variant of spectroscopy made it possible to obtain information on impurity atoms both in the bulk of the sample and in its surface layer.

II. METHOD AND EXPERIMENT

Samples of GaAs p - and n - type doped with zinc growing ($n = 1.6 \cdot 10^{18}$ cm^{-3}) were used as the starting material. Samples in the form of plates were cut from monocrystalline ingots oriented in the <111> direction.

The solubility of iron in GaAs is small (~ 10^{17} at cm^{-3} at 1050^0 C [10]), and therefore, emission spectroscopy was used to take the Mossbauer spectra — the ^{57}Co isotope was introduced into the studied samples, after the decay of which the Mössbauer level ^{57m}Fe is formed.

The NGR spectra were recorded on an electrodynamics-type setup at 295^0 K with a $K_4Fe(CN)_6 \cdot 3H_2O$ absorber. Spectra were recorded twice — before and after removal of the surface layer (~ 150 microns thick).

III. EXPERIMENTAL RESULTS AND DISCUSSION

As already indicated, the concentration distribution of cobalt and iron in GaAsis characterized by two sections – near surface and bulk. The concentration curves are characterized by an increase in the concentration of cobalt in the surface region [9]. In this case, it can be assumed that in the near-surface region enriched in no equilibrium vacancies diffusing from the surface, cobalt interacts with them. In the crystal volume, where the concentration of such no equilibrium vacancies is low, the interaction of cobalt with them can be neglected.

The ^{57}Co (^{57}Fe) NGR spectra for atoms in the near-surface layer (~ 20 microns) depend on the type of conductivity of the initial samples. For n - type samples, they were singlet, somewhat broadened lines, and for p - type samples, they were a quadruple doublet. The results of processing the experimental spectra are shown in the table. Note that the NGR spectra for atoms in the GaAs surface layer are close in their parameters to the spectra given in [11].

After removal of a 150 micron thick layer from the surface of the layer, the NGR spectra changed — they were singlet lines in both n - and p-type samples, but the isomeric shifts were different (see Table 1). In fig. Figure 1 shows the NGR spectra of ^{57}Co atoms (^{57m}Fe) in the bulk of the sample.

Thus, we can conclude that the state of impurity atoms of iron (cobalt) in GaAs depends both on the type of conductivity of the samples and on whether these atoms are in the surface layer or in the bulk of the sample.

Now we consider the charge state and symmetry of the local environment of iron (cobalt) atoms in the bulk of the GaAs. After diffusion doping with cobalt of p-type GaAs samples, they retained whole conductivity, while the whole concentration increased slightly. Because of the diffusion of cobalt, the initial n – type samples also did not change the sign of the current carriers.

As already mentioned, the Mossbauer spectra of the bulk impurity atoms in n - and p - type samples were singlet lines that differ only in the isomeric shift. Apparently, in both cases, impurity atoms are in a cubic environment, and the difference in isomeric shifts is explained by the difference in the charge state of iron.

The values of the isomeric shifts of the ^{57m}Fe NGR spectra in p - type samples are smaller than in n - type samples, which corresponds to a decrease in the electron density on ^{57}Fe nuclei upon transition from p - type samples to n - type samples. This fact can be explained by the fact that a hole in the p - type samples populates the 3d - shell of the iron atom, and thereby the 3d screening of the internal s - electrons decreases, i.e. the transition from p - type samples to n - type samples leads to a change in the electronic configuration of impurity iron atoms from $3d^5$ to $3d^6$ (the process of recharging impurity iron atoms depending on the position of the Fermi level).

Note that, when studying the state of iron impurity atoms in GaAs by EPR [12], the spectra were obtained only for p-type samples. The absence of EPR spectra for n - type samples indicates a charge exchange of impurity iron atoms upon transition from p - type samples to n - type samples. In p-type samples, the EPR spectrum corresponds to Fe^3 + ions with the $3d^5$ (^6S) electronic configuration, while in n-type samples the EPR spectra disappear due to ionization of impurity centers with the formation of the $3d^6$ (^5D) electronic configuration, which in the tetrahedral symmetry field of the EPR spectrum does not give [12]. Thus, there is complete agreement between the results of NGR and EPR spectroscopy.

Table 1.

Isomer shift δ (relative to $K_4Fe(CN)_6 \cdot 3H_2O$ mm / sec.) and quadruple splitting ΔEQ (mm / sec.) Of the NGR spectra of impurity iron atoms in gallium arsenide (at 295^0 K)

Type of conductivity of samples	Fe atoms located in the bulk part of GaAs		Near-surfaceFeatoms	
	δ	ΔE_Q	δ	ΔE_Q
$n = 1,6 \cdot 10^{18}$ см$^{-3}$	0,632	0,10	0,602	0,15
$p = 1,6 \cdot 10^{18}$ см$^{-3}$	0,381	0,10	0,445	0,91

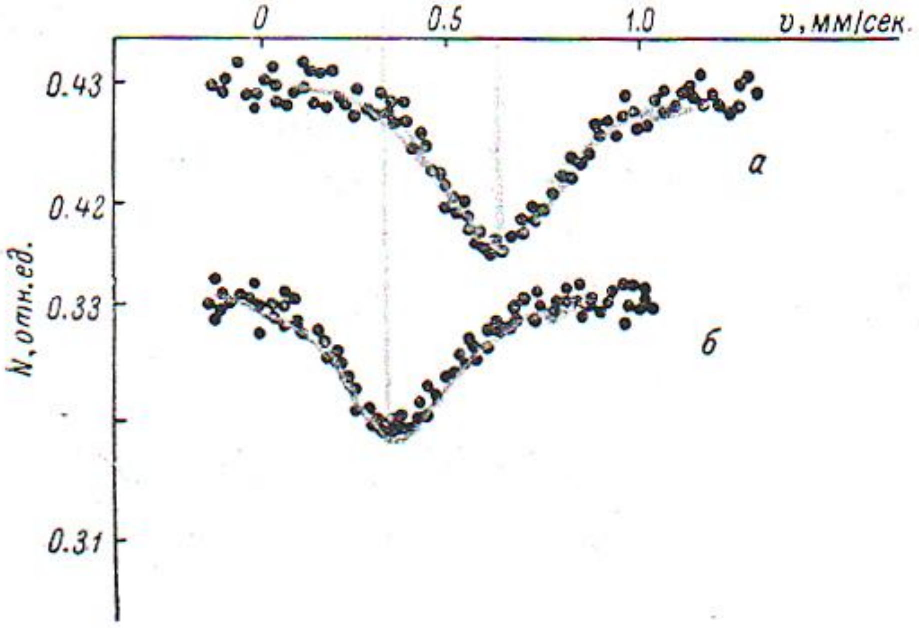

Fig. 1. Mossbauer spectra of 57Co (57mFe) in the bulk of GaAs.a – образец n – типа, б – образец p – типа.

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