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Research Article

TWO-ELECTRON IMPURITY CENTERS WITH NEGATIVE CORRELATION ENERGY

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ABSTRACT

Using the Messbauer spectroscopy method on the 119 Sn isotope, two-electron tin centers with negative correlation energy were identified. It was established that favorable conditions for exchange are realized in PbSe , since for this material the hole concentration is much higher than for PbS.

KEYWORDS

Mixed centers, point defects, negative correlation energy, ionization energy, acceptor satxquadrupole separation, electronic structure, spectra isomer shift.

INTRODUCTION

Ideas about the behavior of impurities atoms in semiconductors are traditional with substitution of an impurity atom for a lattice atom in the band gap of the semiconductor, either a donor or acceptor level is formed, capable of changing position Fermi level give (receive) one electron (so-called single-electron centers).

For the first time, Hubbard [1] carried out a theoretical analysis of the behavior of point defects that can upon interaction with the crystal lattice donate (accept) two electrons (two- electron centers).

In this case, in the band gap of semiconductors, two bands of localized states are formed, separated by the amount of intra-atomic energy (Hubbar energy or correlation energy)

U=E 2 -E 1

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where E 1 and E 2 are the first and second energies ionization center

If U <0 then a level scheme appears, to denote which the terms „d two-electron centers with negative correlation energy or U-centers".

An essential feature of U centers is the instability of their intermediate (singly ionized) charge state. It is energetically favorable for each pair of singly ionized centers to decay into one neutral and one doubly ionized center. In equilibrium, the concentration of U centers in an intermediate charge state is always exponentially (i.e. ~ exp[- U /2 kT]) small compared to their total concentration [2].

Goal of the work

Ideas about the behavior of impurity atoms in polyconductors are traditional: when an impurity atom is substituted for a lattice atom in the band gap of a semiconductor, either a donor or acceptor level is formed, capable of donating (accepting) one electron when the position of the Fermi level changes (the so-called single-electron centers). However, impurity atoms are possible when interacting with a crystal lattice, they give (receive) two electrons (two-electron centers). In the band gap of semiconductors, this is the magnitude of the correlation energy

U=E2 -E1 where E1 and E2 are the first and second ionization energies of the impurity center. If U < 0, then a level scheme arises, which is denoted by the terms "double-electron centers with negative correlation energy or "U centers." An essential feature of U centers is the instability of their intermediate (singly ionized) charge state. Each pair of singly nonionized centers is energetically favorable disintegrate into one neutral and one doubly ionized center. However, despite the successful use of these concepts, two-electron centers with negative correlation energy have not been observed in semiconductors by direct experimental methods. The only exceptions are impurity atoms of tin and germanium in lead chalcogenides and their solid solutions. which by the method of Messbauer spectroscopy on the isotope 119 Sn tic pentras were identified, a model of two-electron donor centers with negative correlation ion energy was proposed, and on its basis all available experiments on the electrical and optical properties of lead chalcagenides doped with tin were explained [1].

METHOD

It should be especially noted that Messbauer spectroscopy is one of the most promising methods for studying the state of impurity atoms in semiconductors. A feature of Mesbauer spectroscopy is the ability to measure in one experiment several hyperfine interaction parameters (isomeric shift, characteristics of the electric field gradient tensor, magnetic field on the nucleus) related to one atom ("Mössbauer probe"). These parameters are determined mainly by the nature and symmetry of the near environment of the Mössbauer probe and, at the same time, they are amenable to theoretical calculation, which makes it possible to directly test the proposed models. The phenomenon of nuclear gamma resonance was discovered in 1958 by R. Mössbauer. Mössbauer spectra are characterized by the following parameters: probability of the effect (Mössbauer factor), spectral linewidth, isomer shift, quadrupole splitting, and Zeeman splitting. The combination of these parameters makes it possible to determine the charge state of the atoms under study, their electronic structure, the symmetry of the local environment, the electric and magnetic fields acting on the probe nucleus, and the vibrational spectra of the matrices.

RESULTS AND DISCUSSION

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To study the process of electron exchange between tin centers in PbS, a sample with the composition Pb 0.06 Sn 0.02 A 0.02 S was chosen.

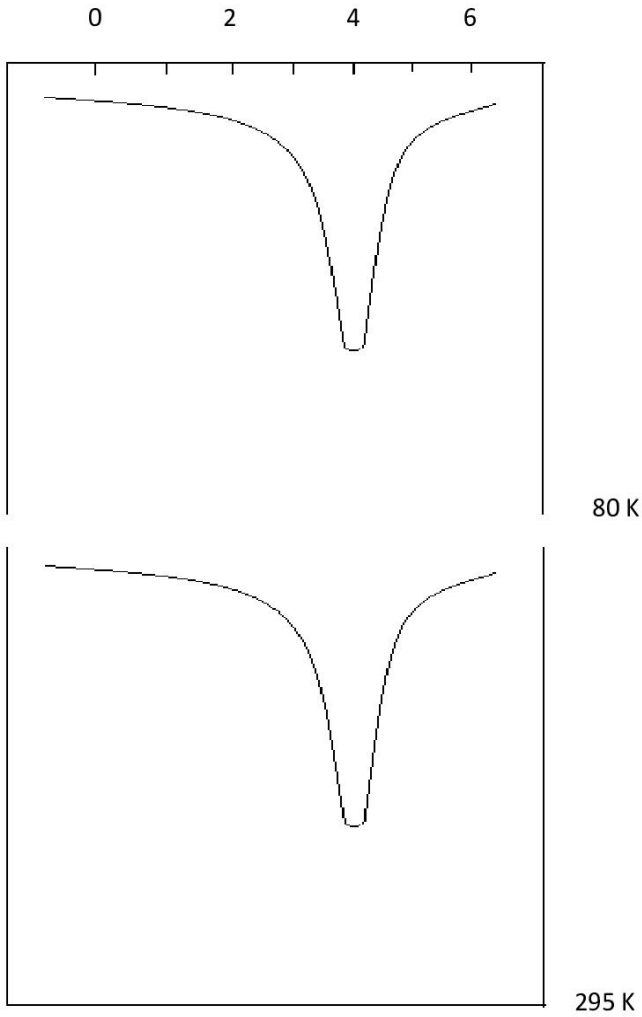

Figure 1

As can be seen from the Mösebauer spectra, in the spectrum of this sample at 80 and 295 K, only **the Sn $^{+2}$ and Sn $^{+4}$ lines were observed**, the isomer shifts of which practically coincide with the isomeric shifts of the known centers **[Sn] ^{0} and [Sn] $^{+2}$** and only a slight convergence of these is observed lines. The convergence of the lines does not depend on the concentration of impurity tin atoms. In other words, in **PbS** the process of electron exchange between the **[Sn] ^{0} and [Sn] $^{+2}$ centers** proceeds much more slowly than

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in **PbSe** . To explain this phenomenon, it should be borne in mind that the rate of electron exchange is controlled by states in the valence band and, obviously, in **P b Se** this process is facilitated due to the fact that the levels of tin **5 S** electrons are located in the valence band. Finally, if one of the stages of charge exchange of tin centers is associated with the capture of a hole, then the most favorable conditions for exchange are realized in **PbSe** since for this material the hole concentration is significantly higher than for **P b S.**

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