

Change in the arrangement of indium atoms in PbTe as a result of increasing the amount of impurity introduced into the crystal

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An Auger-electron analysis of indium-doped lead telluride at an indium doping level ≥ 1 at. % has been performed. Most of the impurity centers introduced into the crystal are in a state with predominantly covalent bonding; this can be explained by the formation of a tetrahedral indium-tellurion coordination.

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Indium-doped lead telluride belongs to that type of solid solutions whose concentration of electrically active impurity centers, after reaching a certain amount of dissolved material in the crystal, remains almost unchanged as more of this material is introduced. The electrophysical properties of the PbTe(In) system have been studied in detail during the past decade.^{1–3} The nonstandard behavior of the indium in lead telluride was attributed to the specific band structure of this system, assuming that a simple isomorphic replacement of lead atoms by indium occurs after the introduction of indium atoms into the crystal.⁴ After analyzing the experimental data of Refs. 1 and 2, we can see that the limiting density of carriers and their mobility depend on the technique used to obtain the doped material.

Auger-electron-spectroscopy method is sensitive to a change in the chemical bond of atoms in different compounds. One reason for this lies in the change of the energy position of the internal electron levels, which results in chemical shifts of the recorded Auger peaks.

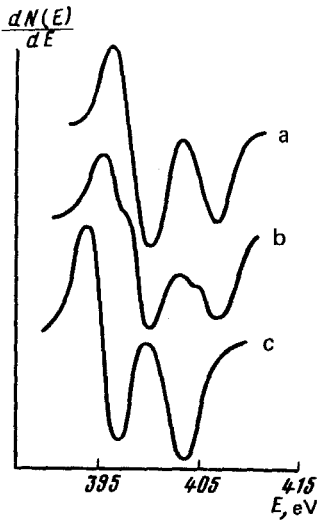


FIG. 1. $M_{4,5}N_{4,5}N_{4,5}$ Auger spectrum of In. a—InP (Ref. 5); b—PbTe(In); c— In_2O_3 (Ref. 5).

Figure 1 shows the obtained $M_{4,5}N_{4,5}N_{4,5}$ Auger spectrum of indium in PbTe. Also shown here for comparison are the analogous In spectra of InP and In_2O_3 .⁵ Indium phosphide is a material with predominantly a covalent bond. In the formation of In_2O_3 the energy position of the In Auger peaks is shifted ≈ 3 eV toward the lower energies; this corresponds to the appearance of bonding with a significant ionic component.

An Auger-electron analysis of PbTe crystals with an indium impurity of more than 1 at.% obtained from a melt showed that most of the indium is in a state with predominantly covalent bonding (Auger peaks at energies $E \approx 400$ eV and 407 eV). The intensity of these peaks, which increases with increasing amount of indium in the crystal, does not depend directly on the carrier density. The peculiarities in the Auger spectrum at $E \approx 398$ eV and 405 eV are attributed to electrically active indium in an octahedral anion environment. Their intensity is almost independent of the amount of indium introduced.

The chemical interaction of metallic impurity atoms with lattice anions is important for compounds with an ionic bonding component, which contain lead telluride. In this case the bonds of the interacting atoms have a tendency to saturate. Under these conditions, the dissolution of the impurity atoms does not lead to their ionization, and the coordination of the nearest neighborhood of the impurity center is different from that the indium atom, which is the substitutional atom. The characteristic indium arrangement in lead telluride is determined by the most probable coordination of tellurium atoms around an impurity center. Such an In-Te bond, which, according to the results of Auger-electron analysis, has an essentially covalent nature, can be realized only when indium is situated in tetrahedral anion vacancies (hybrid sp^3 bond).

It should be pointed out that the carrier mobility decreases with increasing amount of indium in the crystal.² The additional scattering occurs probably because

of the presence of indium impurity centers. Indium in a tetrahedral environment forms a molecular complex, whose formation probability increases with increasing crystallization temperature and impurity concentration.

The results of technological experiments on the growing of PbTe(In) from the vapor phase using tellurium vapors as the transporter gas at different temperatures of the PbTe + In material source favor this assumption. The amount of introduced indium, which was estimated from the partial pressures of PbTe and In, was $\approx 10^{19}$ cm^{-3} . As room-temperature measurements of the conductivity and Hall effect showed, the density of the current carriers increases from 3.7×10^{18} to 8.1×10^{18} cm^{-3} and their mobility increases at the same time from 500 to 960 $\text{cm}^2/\text{V} \cdot \text{sec}$ as a result of the reduction of the source temperature from 920 K to 870 K.

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