INFLUENCE OF CHEMICAL BOND TYPE ON THE LOCALIZATION OF INTERBAND TRANSITIONS IN THE Ge, GaAs, ZnSe, CuBr CRYSTALS

KALUGIN A.I., SOBOLEV V.V.

Udmurt State University
426034 Izhevsk, Russia, sobolev@uni.udm.ru

Выполнены детальные теоретические исследования электронной структуры изоэлектронного ряда кристаллов Ge, GaAs, ZnSe, CuBr. Рассчитаны зоны методом LAPW, общие и парциальные плотности состояний, а также спектры диэлектрической проницаемости методом тетраэдров. Определены локализации оптических переходов в объеме зоны Бриллюэна и их зависимости от природы химической связи кристаллов.

The Ge, GaAs, ZnSe, and CuBr are semiconductors, which are well studied experimentally and theoretically as the model crystals. Their electronic structures are calculated in many papers (see, e.g., [1–3]). These semiconductors form the isoelectronic row from the pure covalent germanium to the ionic crystal CuBr. Therefore it was interested to retrace the changes of their electronic structures. In paper [1] the localizations of interband transitions in two planes of Brillouin zone (BZ) were considered for the Ge. These results show that the optical transitions in Ge are appeared not only at the points of symmetrical lines of BZ, but into the planes ΓKWX and ΓKL too. For the other representative crystals such investigations are not yet carried out.

In our work we calculated the energy structures of the four crystals with the LAPW method [4] within the density functional theory. The dielectric function $\varepsilon_2(E)$ spectra were calculated using the method of tetrahedrons [5] into the 1/48th part of BZ. We also estimated the contributions of each individual tetrahedron for the different pairs of valence and conduction bands in the total curve of $\varepsilon_2(E)$.

The $\varepsilon_2(E)$ spectra of the crystals are shown on the fig.1. Also, there are adduced the partial curves of contributions of transitions between individual pairs of bands (for CuBr it is shown only for first pairs interested in this work). We can see that in $0 - 10$ eV energy range the $\varepsilon_2(E)$ spectra of Ge, GaAs, and ZnSe are analogous. All of three spectra have three main peaks, which are shifted in larger energy when the ionicity of crystals is rised. The intensities of curves are strongly reduced with the energy increase. In the range of most intensive transitions the curves of ε_2 are origined generally by

transitions from two highest valence subbands (V_1, V_2) to two lowest conduction subbands (C_1, C_2). In the case of CuBr, these transitions explain the structures of ε_2 spectrum approximately in the same energy range $0 - 6$ eV. However this crystal is characterized in the larger energy the intensive transitions from the lower lied d-bands of Cu. In other semiconductors they are very small. Also, we can observed that the contribution of $V_2 \rightarrow C_1$ transitions is increased in the row Ge – GaAs – ZnSe – CuBr. At the first, it is caused the decreasing of the width of high valence band; the valence subbands are became more flat.

Besides the integral $\varepsilon_2(E)$ spectra we calculated the localizations of individual transitions in the whole 1/48th part of BZ. It is shown that the transitions are occurred not only at the points of the symmetrical lines of BZ but in the volume they are appeared too. For the Ge crystals our results are well agreed with data of paper [1]. The most transitions for this crystal are occurred generally in the symmetrical planes and lines of BZ. For other crystals we determine that the localizations of transitions are shifted partly into the volume of BZ and this shift is increased in the row of crystals. However this shift is not big as in the strong ionic crystals CdF_2 and CaF_2 [6,7].

So, in this work the important information about the electronic structure and the influence of chemical bond nature on the localization of transitions is obtained. It is shown that the interband transitions are located in the whole volume of BZ. With the increasing of ionicity of materials the localizations are shifted from the symmetrical planes and lines into the volume of BZ.
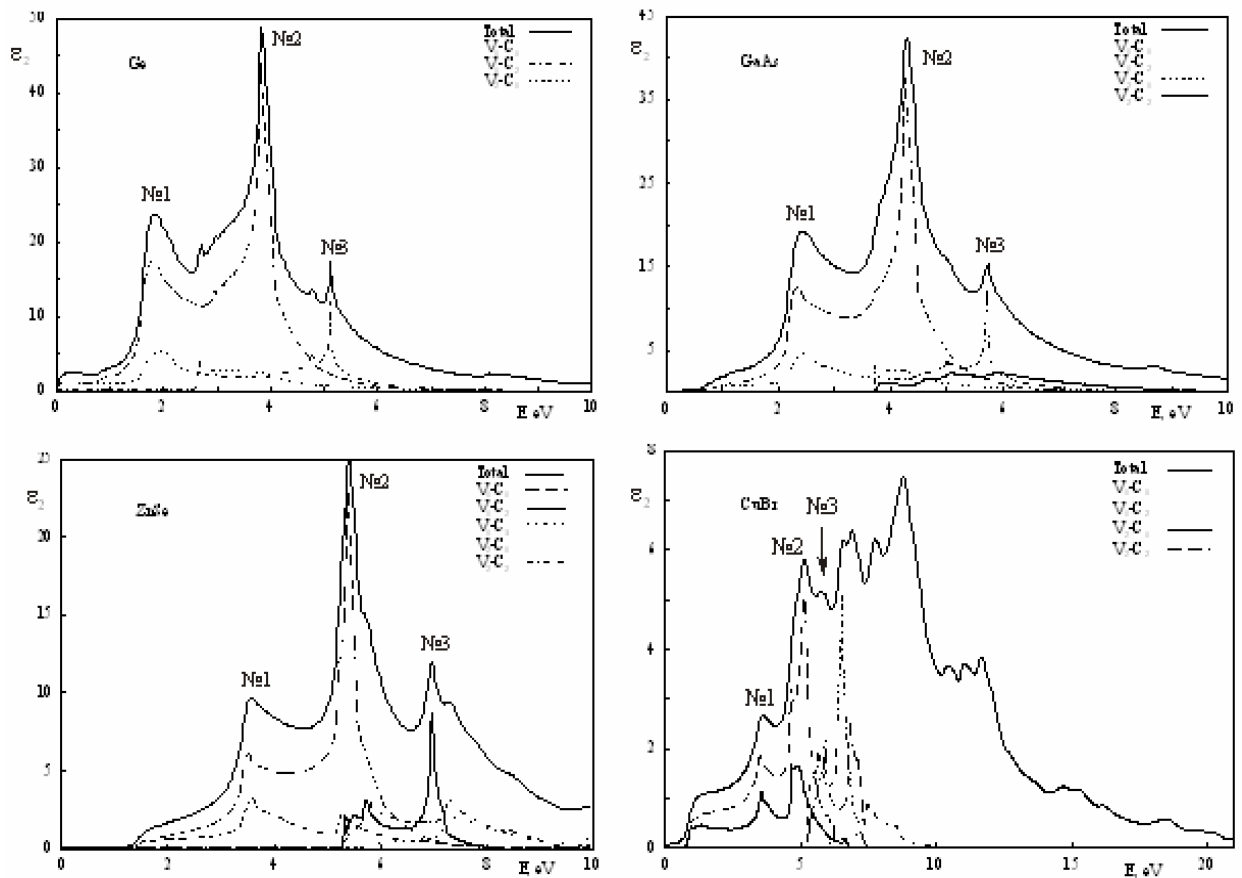
Fig. 1. Theoretical dielectric spectra of Ge, GaAs, ZnSe, CuBr with the partial contributions of transition between individual pairs of bands

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