

Tellurium, sulfur, and oxygen isovalent impurities in ZnSe semiconductor

V.M.Koshkin, A.Ya.Dulfan, N.V.Ganina^{}, V.D.Ryzhikov^{**},
L.P.Gal'chinetskii^{**}, N.G.Starzhinsky^{**}*

National Technical University "Kharkiv Polytechnical Institute",
21 Frunze St., 61002 Kharkiv, Ukraine

^{*}M.Lomonosov Moscow State Academy for Intricate Chemical Technology, 68
Vernadsky Ave., Moscow, Russia

^{**}Institute for Single Crystals, National Academy of Sciences of Ukraine,
60 Lenin Ave., 61001 Kharkiv, Ukraine

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Specific features as formation of doublet and triplet defect complexes ZnSe(D) in ZnSe semiconductor are discussed (where D is tellurium, sulfur, or oxygen). Both elastic and electrostatic interactions of defects have been shown to act symbatically but the latter contribution is more strong. It is shown also that, in contrast to Te doping, sulfur and oxygen impurities result in formation of D–Zn interstitial complexes rather than D-zinc vacancy ones. The triplet defect complexes are of the same composition in all systems but differ in the vacancy, zinc interstitial, and impurity arrangement.

Рассмотрены особенности образования двойных и тройных комплексов дефектов в полупроводнике ZnSe(D), где D — примеси теллура, серы и кислорода, которые замещают Se в анионной подрешетке. Показано, что как упругие, так и электростатические взаимодействия дефектов действуют симбатно, но наибольший вклад вносят последние. Также показано, что в отличие от случая легирования теллуrom, примеси серы и кислорода приводят к формированию не комплексов D-вакансия цинка, а комплексов D-междоузельный цинк. Комплексы с тремя дефектами у всех систем одинаковы, но расположение вакансий, междоузельных атомов цинка и примесей различное.

In [1], thermodynamics of isovalent zinc selenide doping with tellurium was studied and interaction mechanisms of different lattice defects in such crystals were considered. It was shown that, at relatively low concentrations of substituting impurity D in the anion sublattice and depending on the section of the Zn–Se–Te ternary system in which the doping takes place, the dissolution mechanism may differ in principle from the classical one for the substitution solid solution formation relating to the case when ZnSe and ZnTe concentrations are comparable. This is in agreement with data on electron states in ZnSe<Te> studied in [2] as well as with physical mechanisms of

isovalent doping of $A_{III}B_V$ semiconductors [3]. In equilibrium, interaction of defects in ZnSe results in formation of complexes, namely, doublets $\langle \text{Te}, V_{\text{Zn}} \rangle$ (Te being in substitution position in Se sublattice in nearest neighborhood with a vacancy in Zn one) and triplets $\langle \text{Te}, V_{\text{Zn}}, I_{\text{Zn}} \rangle$ (where I_{Zn} is an interstitial zinc ion). At low isovalent impurity concentrations, the complexes are more favorable thermodynamically than isolated Te atoms substituting for Se ones.

When the composition of ZnSe(Te) is deviated from stoichiometry towards Se excess accompanied by V_{Zn} formation, it is just doublets that predominate in equilib-