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Comparative analysis of radiation-induced defect accumulation in $A^{II}B^{VI}$ semiconductors

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A crystallochemical method has been proposed to analyze the accumulation of radiation-induced point defects when estimating the radiation resistance of $A^{II}B^{VI}$ semiconductor compounds. The method makes it possible to compare the radii of absolute instability zones for defects with different interaction potentials and thus the radiation resistance levels of crystals. The knocked-out cation interstitials in $A^{II}B^{VI}$ have been shown to be charged while anions localized in the interstitial positions remain neutral. This results in predominant accumulation of anionic defects, at the same time, however, it is just the cationic defects are most influential on the physical properties of semiconductors.

Предложен кристаллохимический метод анализа накопления радиационных точечных дефектов для оценки радиационной стойкости полупроводниковых соединений $A^{II}B^{VI}$. Данный метод позволяет сравнивать радиусы зон абсолютной неустойчивости дефектов, взаимодействующих с различными потенциалами, и, таким образом, уровень радиационной стойкости кристаллов. Показано, что выбитые междоузельники-катионы в $A^{II}B^{VI}$ заряжены, в то время как анионы, локализовавшиеся в междоузельных позициях, остаются нейтральными. Это приводит к преимущественному накоплению анионных дефектов, но в то же самое время как раз катионные дефекты в наибольшей степени влияют на указанные свойства полупроводников.

Introduction[1]

In [1], the kinetic equations of point radiation-induced defects (RD) have been extended for the multicomponent crystal case under account for the instability zones (IZ), including not only the absolute recombination zones (ARZ) of vacancies v and interstitials i but also the absolute displacement zones (ADZ) of defects of the same sign [3, 4].

This work deals with comparative analysis of radiation resistance (RR) of $A^{II}B^{VI}$ semiconductor compounds, namely, ZnS, ZnSe, ZnTe, CdS, CdSe, CdTe, HgS, HgSe, HgTe, and ZnO. These compounds are similar in their crystal chemistry, exhibit the sphalerite or wurtzite lattice and tetrahedral atomic coordination. All the crystals mentioned show a considerable fraction of binding ionicity, at least 15 to 20 %.

[1]This paper has been written for the Functional Materials issue dedicated to the memory of Prof.Eduard Feliksovich Chaikovsky. Almost all authors had worked near him and were under intellectual influence of his outstanding personality. We were young, he was already among famous scientists, and it was just Eduard Feliksovich who supported the initial investigations in the radiation physics of semiconductors in the Institute for Single Crystals as long ago as in the early 70th. This field of work is in progress still today. In this work, one of its aspects is developed.

In this work, stoichiometric compounds are considered. In analytical expressions for the saturation concentration, C_{sat}, taken from [1], the pre-irradiation defect concentration is taken to be zero. As in [1, 4], ideal single crystals will be considered where RD exit to runoffs (dislocations and block boundaries) can be neglected. The consideration is related to the temperature 0 K, although, as will be shown below, the temperature increase does not impose any additional limitations with respect to small values of the interstitial migration energy, U_m, that is of importance in the IZ model. Strictly speaking, the consideration is related to consequences of irradiation with light particles resulting in formation of single RD. However, as has been shown by Thompson [2], the same relationships are valid for the main features of processes occurring under irradiation with heavy particles, e.g., fast neutrons, if the limiting saturation with point defects is assumed within the cascades. The account for i and ν distribution inhomogeneity within a cascade confirms that result [5].

1. Instability zones and primarily knocked-out atoms

Radii of ARZ and ADZ where two interacting defects may not coexist even at any low temperature or recombine without activation, or become displaced without activation at a very short relaxation time of 10^{-11} to 10^{-10} s, are defined by following expressions taken from [3]:

$$r^{es} = Ze\sqrt{\frac{d}{\varepsilon U_m}}, \qquad (1)$$

$$r^{el} = \left(\frac{3Gd\Delta V_1 \Delta V_2}{U_m}\right)^{1/4}, \qquad (2)$$

where Ze is the ion charge; d, interatomic distance; ε, dielectric constant; U_m, migration energy; G, shear modulus; ΔV_1, ΔV_2, the defect volume change as compared to the size of regular position. The Eq.(1) concerns the Coulomb interaction of defects, Eq.(2), to the elastic one. The equations (1) and (2) have physical sense if the IZ radius exceeds the interatomic distance at least twice or thrice and are defined to a substantial extent by small values if interstitial U_m that is typical of essentially all semiconductors, dielectric, and metal crystals. Note that the IZ size increases when the temperature differs from 0 K, since the i energy increases with respect to the well bottom, therefore, the requirement that U_m should be small becomes less strict [3].

The parameter characterizing the RD appearance, that is, the Seitz threshold of about 25 eV (see [2, 6]) is defined by the lattice atom energy necessary for that the atom leaves its site and becomes fixed in an interstice position. The Seitz threshold is determined by fixation of first RD appearance as the incident particle energy increases. Because of an ARZ presence near each ν, the primarily stabilized RD (PSA) appears only if the formed i exits out of the ADZ of the vacancy that it has leaven. Thus, the determined Seitz threshold corresponds to the kinetic energy of the formed i required for its exit out of the ARZ [3, 7].

The generation of primarily knocked-out atoms (PKA) is defined either by shock mechanisms (above-threshold processes) [2, 6] or by under-threshold mechanisms when the PKA formation is defined by recharging and bond breakdown at the electronic state excitation [7, 8]. No matter what is the formation mechanism, the probability of a PKA exit out of the ARZ is defined by its mean free path length, λ, so that only a fraction of all PKA defined as

$$\eta = e^{-r_0/\lambda} \qquad (3)$$

will leave the ARZ of their vacancies. Of course the λ value depends also on the PKA energy and the crystal characteristics; nevertheless, even (3) itself makes it possible to drawn some conclusions about the RD lot. Estimations using (1) and (2) made in [3] as well the calculations presented below therein show that r^{es} exceeds r^{el} several times, therefore, the path lengths being the same, the probability of PKA exit and formation of observable RD interacting electrostatically within their ARZ is several tens times lower than at their elastic interaction. Thus, it is of primary importance to determine whether the formed PKA charged or no.

It has been shown [3] that, according to the Landau-Zeener criterion [9], already when the ionic bond fraction is very low and the PKA energy is lower than 10^5 eV, the first excited state of PKA is defined by the wave function of almost pure ionic state, therefore, in all $A^{II}B^{VI}$ compounds the nascent PKA are ions. This is confirmed also by consideration of the adiabatic

"stretching" of an ion-covalent bond that results in an increased contribution of ionic wave function [3].

The further lots of cationic and anionic PKA are, however, different. A PKA-anion contains two captured electrons having the detachment energy, E_{ion}, corresponding to the electron affinity one and amounting 2 to 4 eV. As to a PKA-cation in $A^{II}B^{VI}$, two electrons are lost, therefore, E_{ion} of the next electron corresponds to the 3rd ionization potential, thus, 35 to 40 eV for Hg, Cd, and Zn.

According to [2], the PKA energy required for its collision ionization increases as E_{ion}^2. Thus, all other conditions being the same, the detachment probability of excess electrons at anionic PKA exceeds at least 100 times that of further ionization of cationic PKA. Electron capture by charged PKA-cations with kinetic energy at least several tens eV is impossible, since even deep levels of such electrons have energies about 1 eV, the more that the data of [10] show that a considerable fraction of defects has shallow levels, so that essentially all $A^{II}B^{VI}$ with stoichiometry deviations are low-ohmic enough.

It is clear that the PKA-anions are neutral already within their ARZ while PKA-anions are charged. Therefore, according to (1)–(3), the exit probability out of its vacancy ARZ for a charged cation is much lower than for atomic anion, other conditions being the same. This conclusion is confirmed additionally by the fect that even at the same interaction potentials, the IZ of anions is always smaller than that of cations due to lower U_m values of the latter [2, 3, 6].

Thus, the defect formation cross-sections per unit ionizing radiation flux is substantially smaller for PSA-cations than for PSA-anions.

2. *Instability zones and primarily stabilized RD*

We have introduced the term "PSA" bearing in mind that the PSA after exit out of their ARZ will interact with each other ant thus turn out to be unstable, but with longer relaxation times. At not very high temperatures, the separated i and v become stabilized, their annealing activation energy may be considerable. If a PSA i turned out to be in ARZ of an already existing v, it recombines therewith without activation [2]. It has been shown [1, 4] that this effect is amplified due to that RD force the defects of the same sign out of their ADZ into corresponding ARZ, thus accelerating the RD curing process. The contributions of ADZ and ARZ into the accumulation kinetics turn out to be of the same order of magnitude. The expressions (1) and (12) for ADZ and ARZ radii coincide with each other, of course.

The saturation concentration C_{sat} corresponds to the situation when any new RD either appears directly in anyone of accumulated ARZ or, falling into anyone existing ADZ is forced out into the corresponding ARZ. Since under irradiation equal numbers of v and i are formed in the cationic and anionic sublattices, respectively, it is sufficient to determine, e.g., only i concentration. Asymptotic solution of the system of kinetic equations [1] results in the following expressions for C_{sat} of PSA cations and anions:

$$C_1 = \frac{f_{22} + f_{22'} - f_{21}}{(f_{11} + f_{11'})(f_{22} + f_{22'}) - f_{12}f_{21}}, \quad (4)$$

$$C_2 = \frac{f_{11} + f_{11'} - f_{12}}{(f_{11} + f_{11'})(f_{22} + f_{22'}) - f_{12}f_{21}}, \quad (5)$$

where f is the dimensionless IZ volume (the number of atomic volumes in the IZ; the atomic volume is calculated as average one for each binary crystal), while indices denote the radiation-induced defect type generating the respective instability zone (index 1 refers to cation, 2, to anion; primed indices refer to vacancy, non-primed ones, to interstitial). It is seen from (4), (5) that C_{sat} is independent of the RD formation cross-section and depends only on the ratio between the ARZ and ADZ dimensionless volumes.

It is clear from the above that anionic PSA interact with each other as well as with other RD only according to the elastic mechanism while cationic PSA and vacancies interact electrostatically. The elastic interaction of anionic i with cationic ones is defined by the PSA anion atomic radius and that of PSA cations included in the Eq.(2) when calculating ΔV. We do not consider the elastic interaction of neutral cationic vacancies with PSA cations, that corresponds obviously to attraction, since the collapsing of such RD is impossible, the more that such an interaction is estimated to be rather weak. The double-charged cationic PSA interact with cationic vacancies

Table 1. Crystallochemical parameters and values of high-frequency dielectric constant (ε) and shear modulus (G) of $A^{II}B^{VI}$ compounds. r is the radius of cation, anion or void T or O position (lower indices k, a, T and O, respectively). The second lower index i or at refers to ionic or atomic radius, respectively.

	ZnTe	ZnSe	ZnS	ZnO	CdTe	CdSe	CdS	HgTe	HgSe	HgS
$r_{k\,i}$	0.83	0.83	0.83	0.83	0.99	0.99	0.99	1.12	1.12	1.12
$r_{k\,at}$	1.39	1.39	1.39	1.39	1.56	1.56	1.56	1.6	1.6	1.6
$r_{a\,i}$	2.11	1.93	1.82	1.36	2.11	1.93	1.82	2.11	1.93	1.82
$r_{a\,at}$	1.7	1.6	1.26	0.66	1.7	1.6	1.26	1.7	1.6	1.26
$r_{ta}=r_{vk}$	0.652	0.632	0.62	0.568	0.732	0.712	0.7	0.797	0.777	0.765
$r_{tk}=r_{va}$	1.148	1.058	1.003	0.773	1.166	1.076	1.021	1.181	1.091	1.035
r_{oa}	1.079	1.028	0.997	0.866	1.172	1.121	1.089	1.247	1.196	1.164
r_{ok}	1.454	1.35	1.287	1.021	1.5	1.396	1.332	1.537	1.433	1.369
a	6.1	5.67	5.42	4.63	6.48	6.05	5.82	6.47	6.08	5.85
$\varepsilon=n^2$	9.73	6.5	5.92	4.38	7.6	6.63	5.18	15.6	7.16	8.12
G	22.19	26.25	28.88	27.67	19.11	22.36	25.06	13.43	15.19	24.92

by electrostatic mechanism, as well as with each other. To analyze the radiation resistance of $A^{II}B^{VI}$ semiconductor family, it is necessary to establish first of all the values of parameters responsible for IZ size and thus, for the RD saturation concentrations.

3. Crystallochemistry of defects in $A^{II}B^{VI}$

ΔV values are determined in experiment only for few substances using dilatometry and X-ray data [2, 3, 11]. In all cases, interstitials spread the lattice while atoms surrounding ν are shifted towards the vacancy. For calculations using (4), (5) to forecast and compare radiation resistance, an unique system is necessary to estimate ΔV a priori. This system should provide the vacancy size determination, its comparison with sizes of atoms having leaven that position as well as with sizes of particles localized in the corresponding lattice voids. This universal possibility is offered by the crystallochemical closest packing model of spherical ions. The sphalerite structure can be imagined as the closest packing of spherical anions where a half of tetrahedral (T) voids is occupied by cations. In the absence of the latter, the geometric dimension of T-voids in the anionic packing is $r_T^0 = (a\sqrt{3}/4)-R$ and octahedral (O) ones, $r_O^0 = (a/2)-R$ where a is the lattice parameter and R, radius of spheres forming the primary packing (in this case, the anion ionic radius). Of course, when a half of T-voids is occupied by cations spreading the primary packing, the geometric dimensions of free T and O positions are increased, so that their mean dimension takes the value

$$r_T = 0.5R_1 + 0.5\left(\frac{\sqrt{6}}{2} - 1\right)R_2, \qquad (6)$$

$$r_O = \frac{\sqrt{3}}{3}R_1 + \left(\frac{\sqrt{3}}{3} + \frac{\sqrt{2}}{2} - 1\right)R_2, \qquad (7)$$

where R_1 is radius of spheres filling the voids in the primary packing (in this case, cation ionic radii) while R_2, radius of spheres forming the primary packing (in this case, the anion ionic radius) [3].

The void T position has definitely smaller radius as compared to that of the cation in the same position. Let the vacancy radius r_{vk} in the cationic sublattice to be equal to r_T in the anionic packing of the lattice. Both cationic and anionic sphalerite sublattices are crystallochemically symmetric, thus, the sphalerite unit cell can be described equivalently also as a packing of spherical cations where a half of T positions is occupied by anions spreading the initial packing, this time the cationic one. Let us assume that the radiation-induced vacancy radius in the anionic sublattice, r_{va}, is smaller than that of the ion having leaven the corresponding position, just as in the case of r_{vk}. This assumption is in agreement with numerous experimental data [2, 3, 11, 12].

In the Table 1, presented are radii of anionic and cationic ν as well as T and O position radii for different compounds. According to the above, only atomic radii are

Table 2. Saturation concentrations of cations (C_{01}) and anions (C_{02}), the instability zone radii r and relative volumes (f). Lower indices denote the RD type responsible for the corresponding instability zone: 1 refers to cation, 2, to anion, primed indices refer to vacancy, non-primed, to interstitial.

	ZnTe	ZnSe	ZnS	ZnO	CdTe	CdSe	CdS	HgTe	HgSe	HgS
r_{11}	22.16	26.14	26.78	28.79	25.82	26.74	29.68	18.03	25.80	21.26
f_{11}	3425	6795	8255	18184	4621	6142	9430	1390	4843	3025
$r_{11'}$	22.16	26.14	26.78	28.79	25.82	26.74	29.68	18.03	25.80	21.26
$f_{11'}$	3425	6795	8255	18184	4621	6142	9430	1390	4843	3025
r_{22}	11.96	11.15	7.65	1.77	11.59	10.74	7.29	10.43	9.62	7.05
f_{22}	538.5	526.8	192.3	4.23	418.4	397.8	139.6	269.4	250.6	110.4
$r_{22'}$	13.66	12.46	9.94	3.73	13.29	12.06	9.59	12.01	10.86	9.40
$f_{22'}$	801.7	735.99	421.5	39.48	630.3	563.5	317.8	411.3	360.6	261.8
r_{12}	7.14	7.12	6.00	2.93	8.24	8.12	6.80	8.34	8.15	7.43
f_{12}	114.6	137.1	92.89	19.06	150.4	171.8	113.4	137.5	152.6	129.2
r_{21}	7.14	7.12	6.00	2.92	8.24	8.12	6.80	8.34	8.15	7.43
f_{21}	114.6	137.1	92.89	19.06	150.4	171.8	113.4	137.5	152.6	129.2
C_{01}, 10^{-4}	1.3	0.7	0.5	0.2	0.9	0.7	0.4	2.9	0.8	1.6
C_{02}, 10^{-4}	7.5	7.9	16.3	228.8	9.5	10.4	21.9	14.7	16.4	26.9

adopted for PSA anions while ionic ones, for cations. The radius values are taken from tables by Bokiy [13]. In [13], there are no data on oxygen and sulfur atomic radii. We have estimated those values extrapolating the dependence of known atomic radii on the main quantum number for outer electron shells of elements. The linear extrapolation was carried out basing on the multi-interval interpolation. Cubic splines were selected as interpolating function. When extrapolating, the slope of the linear section was assumed to be equal to the first derivative of the spline function at the end of the interval. Basing on that procedure, atomic radii of oxygen and sulfur have been estimated to be 0.66 Å and 1.26 Å, respectively. The plausibility of the values so obtained is evidenced, in particular, by the fact that the value obtained for sulfur coincides with the "covalent" radius in [13] calculated from the molecular spectroscopy data.

Calculations of vacancy size using (6), (7) do not aspire to accuracy but make it possible to carry out a comparative analysis of RD lot in different compounds. Table 2 presents the calculated values of IZ radii and relative volumes for all RD that may contribute to the RD recombination due to their interaction. The v–v interactions are excluded, since their migration energy amounts at least 1 eV, thus, vacancies remain immobile at any interactions with defects. Data on the ionic, atomic, and vacancy radii allow to calculate ΔV initiated by any defect for calculation of the IZ size in (2).

Neither experimental nor calculated data on U_m are known for $A^{II}B^{VI}$. Nevertheless, estimations made by Seitz and Harrington [6] as well as experimental data for numerous metals, graphite, alkali halide crystals, and magnesium oxide show that the U_m for interstitials is of the order of 0.02 to 0.2 eV, U_m values for i-anions exceed those for cations [3, 11]. When calculating the IZ size using (1), (2), we assume U_m = 0.1 eV for cations and U_m=0.2 eV for anions. When calculating r^{es} (1), the high-frequency value $\varepsilon = n^2$ is used where n is the refractive index taken from [13]. When calculating r^{el} (2), the Young modulus E and the Poisson coefficient μ values for ZnSe and ZnS taken from [14] are used to determine the shear modulus $G = E/2(1 + \mu)$. Since we could not find the G values for other $A^{II}B^{VI}$ compounds, we used the known semi-empirical relationship to estimate them. According to that relationship, for isostructural compounds the ratio of shear moduli is close to that of absolute melting temperatures [3]. The values of the latter are taken from [14]. All parameters mentioned are presented in Table 1.

4. Discussion

The above analysis shows that the PSA cations bear a charge while PSA cations are in the atomic state. It seems to be surprising at the first glance that chemically active particles stabilized in the surrounding of the lattice atoms remain unionized and do not enter any chemical binding with their neighbors. Meanwhile, the impurity particles in numerous semiconductors and dielectrics localized in sufficiently large voids of crystal lattice turn out to be in atomic state even under equilibrium conditions [3]. The more probable seems to be that at the "forced" localization of a radiation-induced interstitial, when the whole lattice re-building has no time to occur, the particle remains in the electron state that it had prior to localization in the void position.

The calculations show that the elastic interactions of charged cationic i with other defects are weak due to the cation dimensions are small ($f_{12}<<(f_{11} + f_{11'})$). This makes it possible to simplify the expressions (4), (5) for C_{sat}:

$$C_{01} = \frac{1}{f_{11} + f_{11'}}, \quad (8)$$

$$C_{02} = \frac{1}{f_{22} + f_{22'}}. \quad (9)$$

It follows from (7) that, since PSA-cations are charged and their interaction with cationic i and ν are defined by large Coulomb IZ (1), the PSA-cations may be localized in the PSA state only in interstices between anions. No matter where they are localized, however, they generate the Coulomb IZ, while the IZ of elastic origin is negligible and plays no part at all with respect to C_{sat}. For cations, C_{01} is much less that C_{02} of anions. This is seen from the Table 2 where results of numerical calculations are presented taking into account only recombination processes of PSA, that is, of PKA that have already leaven their IZ. Under account for that the number of PSA being formed from PKA-cations is much less than that from anions (as is shown above), this difference increases additionally. The anionic and cationic defect systems surprisingly turned out to be essentially independent of each other. Thus, the proposed model forecasts that in stoichiometric $A^{II}B^{VI}$ single crystals under high irradiation doses, anionic RD are accumulated in concentrations several decimal orders higher than C_{sat} of cationic RD. An account for the difference of energy transferred to PKA-anions and PKA-cations, at least at shock mechanism of radiation damage due to different PKA masses, may change the concentration ratio by several times, but the orders of magnitudes remain unchanged.

Meanwhile, in the classical work [15], it has been demonstrated reliably that it is just only cationic RD that are found in irradiated ZnSe while in [16], the anionic RD are supposed to form not at all. How this agrees with results obtained basing on the model proposed here ? It has been shown [1] that the presence of pre-irradiation vacancies or interstitials associated with the stoichiometry deviations towards an excess of one component results in changes in C_{sat}. This is one of possible explanations of discrepancy between the model and experiment. Another possible interpretation is that, since anionic RD are neutral atoms, they are difficult to be detected at all and impossible in principle when EPR methods are used taken as the base for conclusions drawn in [15]. Accumulation of neutral interstitial atoms and uncharged anionic vacancies in $A^{II}B^{VI}$ under irradiation can be detected by changes in the electron and hole mobility, appearance of shallow trapping levels thereof and recombination centers in the forbidden gap, by far UV spectra where absorption bands of such atoms may be observed. Generally speaking, neutral defects may influence considerably the lifetimes of excited states, in particular, the luminescence characteristics. The sample microhardness measurements after high irradiation doses are also informative. It has been shown [1] that C_{sat} values characterize the RR properties: the higher C_{sat} is, the lower is RR. The results of this work have shown that two RR characteristics are to be pointed for binary semiconductors, that is, cationic and anionic one (RRC and RRA, respectively). The first exceeds formally the second, but it is just the latter (cationic) RR that may effect considerably stronger on the crystal parameters.

Calculations (see Table 2) evidence that from the viewpoint of anionic radiation resistance (RCA), it is just ZnTe and ZnSe that are best materials while ZnO is the worst one. As to RRC, CdS and ZnO are at the first place while HgTe has the worst resistance. In the sequence of RRA, a trend is observed that sulfides are more resistant

than selenides while those exceed tellurides. An opposite trend can be traced as to RRC: the cationic radiation resistance of MeX compounds increases in the X sequence Te–Se–S–O. No similar sequences can be observed for different cations.

At end, some additional notes can be made. As to lot of atomic *i*-anions that may be localized with equal probabilities in any of four possible void positions of the lattice, that is, in *T* and *O* ones of both cationic and anionic packings: in the *T* position of anionic packing, any anion spreads the lattice. All neutral atoms except for oxygen spread the lattice both in *O* anionic position and in *T* cationic one, while in *O* cationic packing, not only oxygen but also sulfur atoms are smaller than the position geometric dimension. When atoms spread the lattice and generate elastic stresses, this results, as it has been shown, in the saturation effects of the RD concentration. When the localized atoms are smaller than corresponding voids, these atoms do not interact with other ones and become accumulated in the lattice. If the distance between two such atoms approaches the interatomic spacing, formation of S_2 and O_2 molecules is probable, that is, radiolysis of ZnO and sulfides.

As to lot of charged PSA cations localized in the anionic packing voids, three alternatives are possible in general case. First, cations may trap an electron to atomic orbital and become neutral. Second, PSA cations may trap an electron to a deep level. In the third case, the local levels near the cation are shallow, so the electron are free at not very low temperatures. The first case, as we have seen, is excluded. The second one has been studied in [1] and is quite probable under non-equilibrium conditions. Experimental data [10] show, however, that essentially all studied $A^{II}B^{VI}$ crystals with stoichiometry deviations exhibit a very high electronic conductivity in equilibrium. This evidences that at least a substantial fraction of lattice defects gives shallow levels in the forbidden gap. Therefore, it is to demonstrate that a substantial fraction of PSA cations interact in fact electrostatically with each other; their charges are not shielded, since the shallow centers are ionized completely even at moderate temperatures.

Conclusions

1. A method has been proposed for comparative radiation resistance calculation of $A^{II}B^{VI}$ semiconductor compounds taking into account crystallochemical parameters of instability zones of radiation-induced defects.

2. The accumulation of anionic defects under ionizing irradiation has been shown to exceed considerably that of cationic ones; thus, the corresponding saturation concentrations are essentially independent of each other.

3. Within the frame of the model proposed, it has been shown that anionic defects are most probably electrically neutral while the cationic ones bear an electric charge and, as a result, influence much stronger the crystal electrical properties, in spite of their lower concentration.

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Порівняльний аналіз накопичення радіаційних дефектів в напівпровідниках $A^{II}B^{VI}$

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Запропоновано кристалохімічний метод аналізу накопичення радіаційних точкових дефектів для оцінки радіаційної стійкості напівпровідникових сполук $A^{II}B^{VI}$. Цей метод дозволяє зіставляти радіуси зон абсолютної нестабільності дефектів, що взаємодіють із різними потенціалами, і, таким чином, рівень радіаційної стійкості кристалів. Показано, що вибиті міжвузельники-катіони в $A^{II}B^{VI}$ заряджені, тимчасом як аніони, що локалізовані у міжвузельних позиціях, залишаються нейтральними. Це приводить до переважного накопичення аніонних дефектів, тим часом як саме катіонні дефекти найбільшою мірою впливають на зазначені властивості напівпровідників.