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XVI МІЖНАРОДНА КОНФЕРЕНЦІЯ З ФІЗИКИ І ТЕХНОЛОГІЇ ТОНКИХ ПЛІВОК ТА НАНОСИСТЕМ
(присвячена пам'яті професора Дмитра Фреїка)
Матеріали

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(dedicated to memory Professor Dmytro Freik)

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Energy of Substitution of Anions and Cations in Zinc and Cadmium Telluride

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The relevance of the research of point defects is due to their considerable impact on all properties of semiconductor crystals. In this case, to establish the predominant type and the concentration of point defects is necessary to determine their energy creation. These values can be calculated as using the modern quantum chemical programs (GAMESS, Gaussian etc.), and based on the simplified models. Moreover, as it was shown in [1-2], the result, which is obtained on the basis of the semi-empirical method, is sufficient for the interpretation of many experimental data.

Considering the above, promising in terms of the definition of the energy parameters of defects is Harrison's method of connecting orbitals. This method is very simplified, so to get the quantitatively correct values is difficult, but to track the qualitative conformities in the investigated parameters is possible.

In the table is presented the results of calculation of the energy of the substitution defects in ZnTe і CdTe. Based on the data, which are presented in the table, it can be concluded that the halogen atoms are more inclined to substitution of matrix atoms than the atoms of the first group of Periodic Table. In the case of the metals of the first group the energy substitution on cationic and anionic sublattices, are positive, indicating that the disinclination to the formation of defects such as D_{Cd} (D = Cu, Ag, Au). This result may explain the ease of the transitions these atoms between nodal and internodal positions in CdTe, which causes to the time instability of the properties.

Table

Energy substitution (in eV) of cations and anions in zinc and cadmium telluride

	ZnTe		CdTe	
	E (D_{Zn})	E (D_{Te})	E (D_{Cd})	E (D_{Te})
Cu	7.49	34.84	7.92	34.47
Ag	6.28	33.72	6.71	33.42
Au	5.52	32.12	6.02	31.94
Cl	0.15	-1.40	1.40	-1.84
Br	-1.69	-0.88	-0.53	-1.20
I	-3.50	-0.21	-2.34	-0.40

1. I.V. Gorichok. Fizika tverdogo tela, 54 (7), 1373 (2012).

2. I.V. Horichok, H.Ya. Hurhula, V.V. Prokopiv, M.A. Pylyponiuk. Ukr. J. Phys. 61 (11), 992 (2016).