



Topic : Comparative Study Of Stacking Faults In Doped And Undoped Lead Iodide Crystals

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The X-ray investigations of doped and undoped lead iodide crystals shows that the lattice parameters 'a' and 'c' and hence the unit cell volume are sensitively affected by the dopant concentration. Also the stacking faults in doped Lead Iodide crystals are less than the undoped Lead Iodide crystals and goes on decreasing as the concentration of the dopant increases.

Lead Iodide is a direct band gap semiconductor with a layered structure similar to Cadmium Iodide; atoms are located in layers of Pb and I perpendicular to c axis in the succession I-Pb-I-I-Pb-I. Compounds exhibiting a structure of this kind possess a strong intralayer bonding, ionic in nature, between anion and cation. Whereas the anion layers are held together by weak van der Waal's forces (interlayer interaction). On account of weak van der Waal's bonding the cleavage of Lead Iodide normal to the c-axis is very easy. As intralayer and interlayer interaction are different in Lead Iodide crystals, the stacking faults created by slip have different energies. Similarly, the probability of creation of stacking faults by any of the two kinds of slips in different crystals will be different because the stacking fault energy depends upon various factors related to the crystals structure. Table 1 shows the structural data of doped and undoped Lead Iodide crystals.

The energy required to create a unit or partial edge dislocation is proportional to the square of its slip vector. Since the magnitudes of slip vectors of partial and unit edge dislocations in the basal planes of Lead Iodide crystals are $a/\sqrt{3}$ and a respectively, the energies required to create the crystals in doped and undoped Lead Iodide are different (point 1 of table). As the partial dislocations in the basal

planes produce stacking faults, the energy possessed by stacking faults in doped and undoped Lead Iodide crystals were ascending order for increasing dopant concentrations (point 1 of table 1). A unit dislocation may dissociate into two partials bounding a ribbon of stacking fault. The smaller the stacking fault energy, the longer will be the separation between them. It shows that the dimension of the fault, produced by dissociation of a unit edge dislocation in doped Lead Iodide crystals will be in the descending order with increasing concentration of the dopant.

In these crystals there is an ionic binding between cation and anion layers whose magnitudes depends on the distance between two types of ions. If the distance between an anion and cation is less than the sum of their ionic radii, the cation will penetrate into the electron atmosphere of the anion. V.K Agrawal [1] have reported that, under these circumstances, that part of the electron atmosphere, which lies at a greater distance than the cation from the nucleus of the anion exert no force on a charged particle inside it. Hence the force of attraction on a cation will be diminished by its penetration into the electron atmosphere of an anion. Thus, it becomes clear that the force of attraction between two types of ions in doped Lead Iodide crystals decreases, as compared to undoped Lead Iodide crystals, and goes on decreasing as the concentration of the dopant increases. The stacking faults resulting from the slip between anion layers depends upon the van der Waal's forces of attraction between them, whose strength is the function of the mutual deformation of the anions, i.e. of the value of the effective van der Waal's radii of atoms. By comparing 4 and 5 in table 1, it is apparent that coefficient of molecular packing in

undoped Lead Iodide crystals will be higher than doped Lead Iodide crystals. Thus, from the structural consideration, it is concluded that stacking faults in doped Lead Iodide crystals are less than the undoped Lead Iodide crystals and goes on decreasing as the concentration of dopant increases.

The common polytypes of Lead Iodide crystals are found to be 2H. Others less common structures are 4H, 6H, 6R and 12R. As the stacking fault energy in undoped Lead Iodide crystals is less than in doped Lead Iodide crystals, more polytypes should occur in the latter as is also experimentally observed.

The lattice parameters 'a' and 'c' for the doped and undoped lead iodide crystals have been computed from the observed 'd' values by method of successive method of refinement. Mean values are given in Table 1. It may be seen from this table that lattice constants 'a' and 'c' and hence the unit cell volume are sensitively affected by dopant concentration. As seen from Table 1, the lattice parameters 'a' and 'c' for doped lead iodide crystals are increases as the dopant concentration increases. With increase in dopant concentrations, initially the lattice parameters 'a' and 'c' and hence the unit cell volume remains almost constant upto 0.1M. However, at higher dopant concentrations there is a significant change in 'a' and 'c' dimensions of the unit cell and the substitution of dopant ions at cation sites leads to the creation of cations vacancies. The vacancies so created in the lattice may be responsible for the decrease in the coefficient of molecular packing for increasing dopant concentrations as seen from point 4 of table 1.

Sr. No.	Undoped PbI ₂	Doped PbI ₂					
		Al doped (in M.)		Zn doped (in M.)		Cu doped (in M.)	
		0.5	1	0.5	1	0.5	1
1	a-dimension	4.5899	4.6	4.6999	4.6	4.6999	4.599
2	c-dimension	7.0535	7.062	7.1234	7.0535	7.1234	7.0285
3	Distance bet. two anion laye -s (c')	3.28					
4	c/a	0.715	0.713	0.698	0.713	0.698	0.713
5	c/a for ideal h- ex. arrangement of atoms	0.816					

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References

- [1] V.K. Agrawal, Physics Letters A34 (1971) 82