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Impact of the cation and anion vacancies on the optical properties of the tetragonal CdP_2

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Cadmium diphosphide CdP_2 is characterized by a number of unique properties that make it promising for application in optoelectronics [1]. Tetragonal β-CdP_2 belongs to the space symmetry group $P4_12_12$ (D_4^4). In tetragonal CdP_2 each cation (Cd) atom is surrounded with for anion (P) atoms, whereas each anion atom is surrounded with two cation and two anion atoms. In CdP_2 anion atoms form the zigzag chains which penetrate through the crystal. It has been demonstrated that decreasing the bond distance in the phosphorus chain at low temperatures causes an additional amount of anharmonicity of the corresponding modes, which is manifested in more pronounced temperature dependences of their frequencies and damping coefficients [2].

This study is focused on the influence of the cation and anion vacancies on the optical properties of CdP_2 at room temperature. For this purpose series of single crystals of CdP_2 with cation and anion vacancies were obtained by variation of the technological parameters of their growth. We have employed IR and VIS reflectance, as well as Raman spectroscopy to examine properties of obtained samples.

Our results have shown that shape of the bands that correspond to the IR and Raman active phonons are sensitive to the presence of cation and anion vacancies. We also have observed the blue shift of the optical absorption edge due to the presence of the defect levels within the bandgap.

Obtained data provides a direct link between the vibrational and electronical properties of CdP_2 that are crucial for the performance of the devices based on studied compound.

1. *Marenkin, S.F., Trukhan, V.M.*, Phosphides and arsenides of Zn and Cd. // IP A.N. Varaksin.-2010. -223.
2. *Shportko K. V.* How the phosphorus chains impact on the vibrational properties of diphosphides ZnP_2 and CdP_2 at low temperatures. // Semiconductor Physics, Quantum Electronics & Optoelectronics.-2016. **-19**, N 4.-P. 377-383.