Theoretical study for structural stability and electronic properties induced by various point defect of KDP and ADP crystals

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The potassium dihydrogen phosphate (KH_2PO_4, KDP) and its analog crystal ammonium dihydrogen phosphate ($NH_4H_2PO_4$, ADP) are excellent nonlinear optical crystal for widespread application. [1-4] The two crystal both possess similar structures and high damage threshold. However, these optical elements are seriously damaged by ultraviolet laser irradiation in the current application, and the actual damage threshold is far lower than its theoretical value, severely reducing the service life of the components. Defects are considered as the most related issue affecting the damage threshold, such as point defects and cluster defects.[5-7] The mechanism of specific defects on the properties and on the microscopic stress for KDP and ADP crystals are not very clear yet. Moreover, the different internal origins of the damage threshold between KDP and ADP crystals are not well understood due to the limitation of the experiment method.

In this work, combined with some experiment method, such as positron annihilation technique and Raman spectra, the optical absorption properties and the mechanism of microscopic stress induced by point and cluster defects were studied systematically based on the first-principle method. Through the study, the oxygen defect could make the formation of H_2O to affect the structural stability, while the Fe^{3+} impurity defect caused large and broad optical absorption peaks near 200-300 nm to reduce the damage threshold. Besides, the ADP crystal possess the relative stronger hydrogen bond to maintain the stability of the microstructure to make higher damage threshold. It is vital significant to improve the quality of the crystal and promote the application of KDP and ADP crystals.

References

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