

First-principles study of charge states of point defects in Ti:sapphire co-doped with nonisovalent atoms

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Ti ions in titanium-doped sapphire may exist in different charge states and demonstrate a tendency to form pairs, triples and larger defect clusters [1,2]. The laser efficiency of Ti:sapphire is affected by a residual infrared absorption in the emission band of the Ti:Al₂O₃ laser. The residual absorption is caused by Ti³⁺-Ti⁴⁺ pairs. In this connection, the reduction of the ratio of the concentration of isolated Ti³⁺ defects to the concentration of Ti³⁺Ti⁴⁺ pairs is a challenge problem.

We analyze the role of co-doping in a control of the charge state of Ti in Ti:sapphire and an influence of co-doping on the formation of Ti–Ti pairs. We consider co-doping with carbon, nitrogen and fluorine. The analysis is based on the density function theory approach implemented in the open-source DFT-package SIESTA [3].

It is found that carbon defects have high formation energy and do not affect the charge state of Ti defects. In view of low formation energy of substitutional N_O⁻ defects, co-doping with nitrogen yields negative effect: the concentration of Ti³⁺-Ti⁴⁺ pairs increases. In contract, co-doping with fluorine atoms that form F_O⁺ defects may result in an essential decrease of the concentration of Ti³⁺-Ti⁴⁺ pairs. We determine the conditions at which a large ratio of Ti³⁺ to Ti³⁺-Ti⁴⁺ can be achieved.

The band structure of Ti:sapphire co-doped with fluorine is calculated. It is established that co-doping with fluorine does not result in an appearance of additional impurity levels in the band gap, and, therefore, fluorine admixtures do not influence optical properties of Ti:sapphire.

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