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Theoretical study of defect structures in pure and C, Mg-doped aluminum oxide (Al2O3)

Abstract
The stimulated luminescence features of aluminum oxide (Al2O3) regulated by defects and impurities within the structure are well-known. Examples of resultant applied materials include Al2O3:C and Al2O3:C,Mg. This study examines the basis for the experimental observation that doping Al2O3 with Mg and C improves its thermoluminescence (TL) sensitivity. In order to study the electronic structures and formation energies of point defects in pure and C, Mg doped Al2O3, first principles plane wave pseudopotential calculations were carried out. Using density functional theory as a tool, we systematically investigated the geometry and electronic structure of Al2O3 both in the presence and absence of individual dopant elements as well as in the presence of defect combination. According to the current study, the chemical environment has an important effect on the relative defect formation energy for doping with individual elements or in combination. We find that when an individual dopant element is present, the requirements for a good TL dosimetry material such as electron trapping, hole trapping and luminescent centers are satisfied. Interestingly, a simultaneous presence of the two dopant features also satisfies this need. It is observed that each dopant element contributes differently to the formation of several kinds of trapping centres. The underlying mechanism of the TL process in (Mg, C) doped Al2O3 was also investigated.

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