

Atomistic Simulation of Origin and Local Structure of Reidinger Defects in $\text{Ba Mg Al}_{10}\text{O}_{17}$

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Barium magnesium aluminate in the β -alumina structure is the host for a Eu^{2+} -activated blue phosphor (BAM) used in fluorescent lamps and display applications. Unlike the red and green phosphors used in the tri-phosphor blends, this phosphor is relatively unstable during the lamp life, and leads to undesirable color shifts with time. Generation of color centers during the lamp life is believed to be a dominant mode of degradation of this phosphor.

The Reidinger defects are believed to be a source of color centers in similar aluminates with β -alumina structure. These defects could lead to generation of F^+ and F type color centers by ultraviolet radiation and bombardment of energetic particles from the discharge. The absorption bands of the F and F^+ centers overlap with 254 nm radiation from the Hg-discharge and thus, affect the performance of this phosphor. This presentation explores the geometry and origin of the Reidinger defects in BAM.

Using an atomistic simulation package, "SHELL",¹ I have studied how the Reidinger defects could be formed in the intermediate plane of the BAM lattice. Two cases have been explored in detail. One is related to the presence of point defects (Al_{Mg}^+). This could lead to isolated Reidinger defects in the BAM lattice. The other is related to a solid solution of $\text{Ba}_{0.75}\text{Al}_{10}\text{O}_{17.25}$ (Phase I) and $\text{BaMgAl}_{10}\text{O}_{17}$ (BAM). The Reidinger defects are intrinsically present in Phase I of Ba hexaaluminate (BAL). Thus, a solid solution of BAL and BAM is expected to contain the Reidinger defects. Both the cases considered in this study could result from a lack of stoichiometry in the input composition.

SHELL implements a lattice dynamics approach within a quasi-harmonic approximation of interatomic potential. Within this theoretical framework, the program computes various thermodynamic potentials, optimized geometries and associated structural properties of ionic crystals. Before using this approach to simulate the defect structure of BAM, the program was first tested for its reliability in predicting crystal structures and cohesive energies of Al_2O_3 , MgO , and BaO . Assuming a quasi-periodicity in the presence of point defects, a supercell approach was utilized for studying the stability and geometry of the Reidinger defects in BAM.

For both the cases, the calculated structural modifications of the lattice surrounding a Reidinger defect are in excellent agreement with those determined for BAL from the diffraction measurements.² The structural modifications surrounding the Reidinger defect will be discussed during the presentation. An analysis of the changes in Gibbs free energy due to the Reidinger defects will be made to illustrate how these defects could come to exist in the BAM lattice.

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1. M. B. Taylor, G. D. Barrera, N. L. Allan and T. H. K. Barron, Phys. Rev. B 56, 14380 (1997).
2. S. R. Jansen, Alkaline-earth Aluminum Oxynitride with the β -alumina or the Magnetoplumbite Structures (Ph. D. Thesis, Technische Universiteit Eindhoven, 1998).