Conference Abstract

Defects and dopants in Anorthite ($CaAl_2Si_2O_8$)

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Abstract

Calcium aluminosilicate, $CaAl_2Si_2O_8$, is a promising economically important ceramic material that has found applications in several areas, such as glass production and petrology [1-2]. Atomistic scale simulation techniques are used to study the intrinsic defects and doping behaviour in $CaAl_2Si_2O_8$. The cation anti-site defect, in which Al and Si ions exchange their positions is the most favourable defect agreeing well with the experimental observation [3]. The O-Frenkel, which is necessary for the formation of O vacancies in vacancy-assisted O-ion diffusion, is the second most favourable defect. The Ca-Frenkel is higher in energy only by 0.62 eV than the O-Frenkel implying that this defect would be also observed. Prominent isovalent dopant on the Ca site is the Sr. The formation of Ca interstitials required to enhance the capacity of this material and oxygen vacancies are favoured by Fe^{3+} doping on the Si site. The favourable tetravalent dopant on the Si site and the Al site to form Ca vacancies is the Ge. The results presented herein can motivate further experimental work for the development of $CaAl_2Si_2O_8$.

Keywords: Anorthite, Defects, Dopants, Atomistic simulation.

References

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