

X-ray and Neutron Diffuse Scattering by Cation and Anion Deficient Zirconia

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Zirconia, ZrO₂ doped with cations (e.g. Y³⁺, Sc³⁺, Ca²⁺), is a technologically important material, e.g. with respect to its high ionic conductivity based on oxygen vacancies. An alternative route to create the vacancies is the doping with anions (e.g. nitrogen). To understand the properties of these materials it is necessary to know both long-range and short-range ordering effects of cations, anions and vacancies as well as relaxations of atoms surrounding the defects. The diffuse scattering of zirconia with different types of cation dopants with or without co-doping with nitrogen has been investigated by neutron and X-ray scattering. The typical neutron diffuse scattering of cubic stabilized zirconia shows diffuse maxima being part of global features, such as diffuse bands perpendicular $\langle 111 \rangle$, whose distance corresponds to the smallest Zr-O distance. This can be described by a defect model based on statistically distributed vacancies surrounded by radially displaced ions [1], ascribed to rhombohedral short-range order. The parameters of this model, i.e. the various amounts of the displacements of the ions, are obtained by fitting them to the experimental data and are compared to theoretical (ab initio) predictions.

[1] Kaiser-Bischoff I., Boysen H., Frey F., Hoffmann J.-U., Hohlwein D., Lerch M., *J. Appl. Cryst.*, 2005, **38**, 139-146.

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