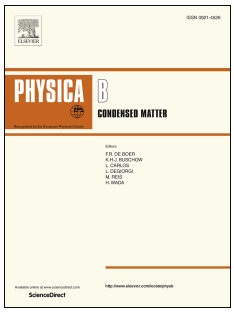
Accepted Manuscript



A theoretical model of lattice diffusion in oxide ceramics

E.S. Smirnova, V.N. Chuvil'deev, A.V. Nokhrin

PII: S0921-4526(18)30443-5

DOI: 10.1016/j.physb.2018.06.043

Reference: PHYSB 310951

To appear in: *Physica B: Physics of Condensed Matter*

Received Date: 28 March 2018

Revised Date: 28 June 2018

Accepted Date: 29 June 2018

Please cite this article as: E.S. Smirnova, V.N. Chuvil'deev, A.V. Nokhrin, A theoretical model of lattice diffusion in oxide ceramics, *Physica B: Physics of Condensed Matter* (2018), doi: 10.1016/j.physb.2018.06.043.

A theoretical model of lattice diffusion in oxide ceramics

E.S. Smirnova, V.N. Chuvil'deev, A.V. Nokhrin*

Lobachevsky State University of Nizhny Novgorod, 603950, Nizhny Novgorod, Russia

E-mail: nokhrin@nifti.unn.ru

Abstract

The authors propose a phenomenological description of volume diffusion in oxide ceramics. The paper considers vacancy and non-vacancy mechanisms of diffusion. In vacancy models, ion migration is described as a fluctuation with formation of a "liquid" corridor that facilitates diffusion transfer of ions through the melt or a fluctuation with formation of a "hollow" corridor where ion movement is activation less. Non-vacancy models concern a fluctuation with formation of a liquid spherical area of a size that corresponds to the first coordination sphere. It has been demonstrated that the vacancy models are fit for cubic metal oxides and the non-vacancy model works well to describe diffusions in non-cubic oxides. The developed modes have been rigorously compared against experimental data, which revealed that diffusion activation energies of metal ions and oxygen ions calculated using the proposed models are in good agreement with the published values for volume diffusion in stoichiometric oxide ceramics.

Keywords: diffusion, oxide ceramics, crystal structure

1. Introduction

Diffusion in ceramic materials is among the matters of current interest [1-24]. One of the reasons for that lies in the development of new technologies for the production of nano- and ultrafine-grained ceramic materials [1-3], the diffusion processes in which (diffusion "dissolution" of pores, grain growth, phase transformations, etc.) during sintering play a dominant role. As for

* Corresponding author (Nokhrin@nifti.unn.ru)