Accepted Manuscript

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PII: S0921-4526(18)30443-5

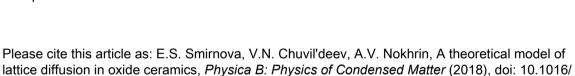
DOI: 10.1016/j.physb.2018.06.043

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

j.physb.2018.06.043.



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A theoretical model of lattice diffusion in oxide ceramics

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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

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