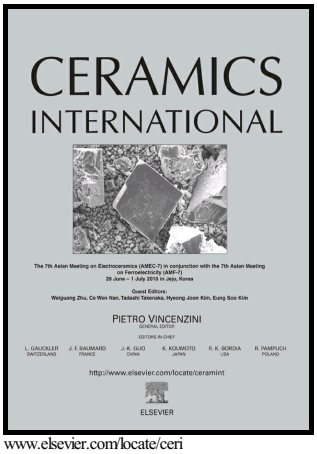
Author's Accepted Manuscript



www.elsevier.com/locate/ceri

Effect of Oxygen Vacancy and Temperature on the Lattice Parameters of Mullite Using a Novel Bridging Cell Multiscale Method

Seyed Mohammad Mahdi Zamani, Kamran Behdinan

PII: S0272-8842(17)31303-2
DOI: http://dx.doi.org/10.1016/j.ceramint.2017.06.085
Reference: CERI15607

To appear in: *Ceramics International*

Received date: 28 October 2016
Revised date: 13 June 2017
Accepted date: 14 June 2017

Cite this article as: Seyed Mohammad Mahdi Zamani and Kamran Behdinan Effect of Oxygen Vacancy and Temperature on the Lattice Parameters of Mullite Using a Novel Bridging Cell Multiscale Method, *Ceramics International* http://dx.doi.org/10.1016/j.ceramint.2017.06.085

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting galley proof before it is published in its final citable form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

ACCEPTED MANUSCRIPT

The Effect of Oxygen Vacancy and Temperature on the Lattice Parameters of Mullite Using a Novel Bridging Cell Multiscale Method

Seyed Mohammad Mahdi Zamani, Kamran Behdinan
Advanced Research Laboratory for Multifunctional Light Weight Structures, Department of Mechanical & Industrial Engineering, University of Toronto, Toronto, Canada

ABSTRACT

This study applied a novel Bridging Cell Method (BCM) multiscale modeling technique to identify the internal energy and lattice parameter variations of mullite with respect to the oxygen vacancy content of its structure, at temperatures ranging from 300K to 1500K. The BCM model decomposed the system into three domains: continuum, bridging, and atomistic. Temperature-dependent numerical calculations were then applied to solve the systems of equations. Next, the supercells of mullite were generated by removing oxygen atoms from a silimanite crystal structure and replacing the Si with Al atoms. Such replacements occurred in the atomistic domain where interatomic and temperature-dependent potential functions were used to obtain the internal energy and lattice parameter variations of the mullite family as a function of the structure's temperature and oxygen vacancy. The results were validated at different temperatures via applicable experimental data previously reported in the literature. At all temperatures, the results indicate a linear relationship between the internal energy/cell of mullite and the oxygen vacancy factor. Lattice parameter a was found to linearly increase as the oxygen vacancy increased, whereas the b and c lattice parameters nonlinearly reduced or increased, respectively. Furthermore, in all cases, a temperature elevation led to a linear increase in the lattice parameter since the thermal expansion coefficient was found to be positive in all three directions. The results indicated that the main origin of lattice parameter fluctuations in the mullite family is the rotation of the structure *around* the c-axis, which is attributable to the removed oxygen atoms hence, there is a longer bond length of Al-O as compared to Si-O. *Additionally*, the thermal properties of mullite including variations in *the* internal energy and lattice parameter fluctuations with respect to temperature, are independent of the composition. This validated BCM mullite model can be used for structural analysis at higher temperatures.

Keywords: Multiscale Modeling, Mullite, Bridging Cell Method, Lattice Parameter, Internal Energy

1. Introduction

Accepted manuscript

Download English Version:

https://daneshyari.com/en/article/5437522

Download Persian Version:

https://daneshyari.com/article/5437522

Daneshyari.com