Final Report Prepared for the U.S. Department of Energy

Project Information:

Project title: Structural Transformations in Ceramics: Perovskite-Like Oxides and Group III, IV, and V Nitrides

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Budget Period: August 1, 2003 – January 31, 2008

Recipient Organization: Auburn University, Office of Sponsored Programs, 310 Samford Hall, Auburn University, Auburn, Alabama 36849-5112

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Project Overview:

This project is a theoretical investigation of mechanisms of reconstructive structural transformation in main group oxide and nitride ceramics. My group is in close collaboration with Dorian, Lewis, and Stokes at Brigham Young University, who are also funded by the DOE in a related project. The primary goal of this project is establish more quantitative understanding of mechanisms of reconstructive structural transformations and to better predict formations and structural stability conditions in ceramic nitrides. Our studies are carried with an innovative computational approach that combines systematic group-theoretical analysis of all the possible homogeneous transformation pathways with quantitative first-principles total energy calculations. During this project period, we have investigated the transformation pathways of the B1-to-B3 transition in NaCl and PbS, the Zincblende-to-Rocksalt transition in SiC, and the wurzite-to-Rocksalt transition in GaN and AlN, the corundum-to-Rh2O3-II transition in Al2O3, the meta-stable beta-to-delta phase transition in Si3N4. In addition, we also carried put theoretical predictions of high-pressure polymorphisms in P3N5, and Gallium oxy-nitrides, the T-P phase diagrams in Si3N4 and Ga2O3, and lattice anharmonicity in MgO. We have published 7 journal papers based o the research support by this grant, and we will submit two more manuscripts in the near future, and are preparing one manuscript. The PI and his graduate students have made many invited and contributed conference presentations. One graduate student, Dr. Bin Xu, was partially supported by this grant, and he received his Ph.D degree in Physics from Auburn University in August 2009.

Highlights of Research Results:

Here we highlight a few of our research accomplishments during the current budget years. More details can be found in our publications listed in the next section.

(1) We proposed a general bilayer-sliding mechanism for the phase transitions from the tetrahedrally bonded B3 or B4 structure to the octahedrally bonded rocksalt structure. We have demonstrated in various materials systems (SiC, GaN, and AlN) that this series of pathways are the only energetically favored pathways.

(2) We proposed a novel single bond-breaking-and-reforming mechanism for the corundum-to-Rh2O3-II phase transition in Al2O3. We furthered predicted the meta-stability of the two phases in Al2O3. This is likely a general transformation pathways for all the A2X3 type of compounds.

(3) We have predicted several dense group-VB nitrides and group-IIIB oxy-nitrides that can be synthesized at the high-pressure conditions.

(4) We have predicted the solid state T-P phase diagrams of SiN3 and Ga2O3.

(5) We have developed an efficient numerical technique to evaluate 3rd order lattice anharmonicity of crystals. This is the first step to go beyond quasi-harmonic approximation to predict vibrational entropy in solids.

Publication:

1. Bin Xu, Jianjun Dong, H. Stokes, and D. Hatch, "Transformation pathways for the wurtzite-to-rocksalt phase transition in AlN", in preparation.

2. Bin Xu, Jianjun Dong, and H. Stokes, "First-principles study of kinetic barrier and metastability for the corundum-to-Rh2O3-II transition in Al2O3", to be submitted to PRL.

3. Bin Xu, Jianjun Dong, and P.F. McMillian, "First-principles study of phase transitions in silicon nitride at high-pressure", to be submitted to PRB.

4. Xiaoli Tang and Jianjun Dong, "Pressure dependence of harmonic and anharmonic lattice dynamics in MgO and implications to lattice thermal conductivity", Phys. Earth Plan. Inter. 174 , 33-38 (2009).

5. H.T. Stokes, J. Gunter, D.M. Hatch, Jianjun Dong, H. Wang, and J.P. Lewis, "*Bilayer siliding mechanism for the Wurtzite-to-Rocksalt transition*", Phys. Rev. B 76, 012102-1-4 (2007).

6. D. Machon, P.F. McMillan, Bin Xu*, and Jianjun Dong, "A high-pressure study of the β-to-α transition in Ga2O3", Phys. Rev. B 73, 094125 (2006)

7. E. Soignard, D. Machon, P.F. McMillian, Bin Xu*, Jianjun Dong, and K. Leinenweber, "*Spinel-structured gallium oxynitrides (Ga3O3N) Synthesis and Characterization: an experimental and theoretical study*", Chem. Mater. 17, 5465 (2005).

8. D. Hatch, H. Stokes, Jianjun Dong, J. Gunter, H. Wang, and J. Lewis, "*Bilayer sliding mechanisms of zinc-blende to rocksalt transition in SiC*", Phys. Rev. B 71, 184109 (2005).

9. H. Stokes, D. Hatch, Jianjun Dong, and J. Lewis, "*Mechanisms of phase transition between the B1 and B2 structure types in NaCl and PbS*", Phys. Rev. B 69, 174111 (2004).

10. Jianjun Dong, A.A. Kinkhabwala*, and P.F. McMillan, "*High-pressure polymorphism in phosphorus nitrides*", Phys. Stat. Solid. B 241, 2319 (2004).

Major Participants (August 1, 2003 – January 31, 2008):

Name	Title /Affiliation	Budget
Dr. Jianjun Dong	Associate Professor Physics Department Auburn University	Dong is the project principle investigator. He is responsible for overseeing the operation of the whole project, developing new algorithms for calculating the complex enthalpy landscapes, carrying out first-principles calculations, and communicating with collaborators including the theorists at BYU and the experimentalists at UCL (London, UK)
Mr. Bin Xu	Graduate research assistant, Physics Department, Auburn University	Xu was partially supported as aGRA through the rest of the project period. The research work of this project was a major portion of his Ph.D thesis. He finished his thesis defense in August 2009.