

PAPER REF: 6452

## **ATOMISTIC MODELING AND STRENGTH CALCULATIONS OF Ni-Al SUBMICRON AND NANOSIZED COMPOSITES**

**Alla V. Balueva<sup>1</sup>, Ilia N. Dashevskiy<sup>2</sup>**

<sup>1</sup>University of North Georgia, Mathematics Department, P.O. Box 1358, Gainesville,  
Georgia, 30503, USA

<sup>2</sup>Institute for Problems in Mechanics of Russian Academy of Sciences, pr. Vernadskogo 101, 1,  
Moscow, 119526 Russia

(\*)Email : alla.balueva@ung.edu

### **ABSTRACT**

The present work is an experimental and theoretical approach to synthesize and characterize Ni-Al submicron and nanosized composites reinforced by epoxy and carbon nanotubes. We should develop a molecular dynamics potential first for Al + Ni reaction, and then validate calculations with the experimentally obtained mechanical and energetic properties of the fabricated bulk nanosolids. The model will be developed and the calculations will be made to obtain the mechanical strength of the materials from the Ab-initio calculations.

**Keywords:** atomistic modelling, energetic structural materials, strength calculations.

### **INTRODUCTION**

The binary energetic materials are of significant interest because of their capability of releasing heat during chemical reaction. On another hand this type of materials provides an opportunity to develop dual functional materials with both strength and energetic characteristics. When mixtures like nickel and aluminum are synthesized at nanoscales, their mechanical strength can be increased because of the nanostructure, while their energetic characteristics are also improved significantly. These dual functional materials also have dual branches of failure criteria. One is the strength based failure criterion. The second is the reaction based failure criteria that implies that chemical reaction should not initiate when only strength is desired. However, a complete chemical reaction should take place when needed. It is thus, essential that mechanisms of chemical reaction and strength on atomistic level were understood. For atomistic modeling and abinitio first principles calculations we are using Density Functional Theory (DFT) and Molecular Dynamics (MD).

Binary energetic materials are also of significant interest because of their capability to release substantial amount of heat during a chemical reaction together with their relative low insensitivity. A further issue of interest is the properties of binary energetic materials mixed with appropriate reinforcements. Using such reinforcements provides the dual functionality of structural strength along with the energetic properties. Among these, micron, submicron, and nanostructured composites have been the object of thorough investigation both in the field of numerical simulation and experimentation. First, we should develop a molecular dynamics potential for Al + Ni reaction, and then for the mixture, Al + Ni +C, and validate both with the experimentally obtained mechanical and energetic properties of these materials.

## RESULTS AND CONCLUSIONS

On the base on Quantum Mechanics approach the transition states are viewed as saddle points of the first order on the potential energy surface. The difference between energies on the top of the saddle point and on the minimum on potential energy surface (a stable state, e.g. for the reactants) is an activation energy of the reaction, calculation of which is one of our primary goals.

When considering Al and Ni reaction, significant improvement should be done for MD to be applicable for simulation of complex materials consisting of two or more crystals systems. The main question before MD running is how to calculate interatomic potentials: exactly from DFT (some restrictions for calculation time due to the computer capacities and as a consequence it's possible to catch up only the beginning of the reaction) or through fitting interatomic potentials (analytical expression and therefore the calculation time is several order less, but a lot of preliminary analytical work before calculations) (e.g. Pun & Mishin, 2009).

Crystallographic experiments show that it is most likely the preferred final configuration of AlNi compound after the reaction is B2 structure, with Ni atom in the center. The fact that the melting temperature for Al is lower than for Ni gives the idea that possible mechanism of the Al/Ni reaction is liquid/solid type, which means atoms of Ni diffuse into solute of liquid Al after melting. In this scenario the number of atoms of Al is greater than the number of Ni atoms, therefore this mechanism leads to formation of Al<sub>3</sub>Ni compound, which is L21 structure. While choosing the potentials this fact should be taken into account.

Calculations for Al and Ni reactions will be made to understand at which temperatures the reaction starts for different pressures, and what the release of heat for different temperatures and pressures. Also, the model will be developed and the calculations will be made to obtain the mechanical strength of the materials from the Ab-initio calculations.

## REFERENCES

- [1]-Liang Chen, David S. Sholl, and J. Karl Jonson. First Principles Study of Adsorption and Dissociation of CO on W(111). *J. Phys. Chem. B* 2006, 110, 1344 - 1349.
- [2]-Andreas Eicher. CO oxidation on transition metal surfaces reaction rates from first principles. *Surface Science* 498 (2002) 314 - 320.
- [3]-Geun Ha Ryu, Seung C. Park, Soon-Bo Lee. Molecular orbital study of the interactions of CO molecules adsorbed on a W (111) surface. *Surface Science* 427 - 428 (1999) 419 - 425.
- [4]-G.P. Purja Pun and Y. Mishin, "Development of an interatomic potential for the Ni-Al system," *Phil. Mag.* 89, 3245 (2009).
- [5]-Granier, J.J., and Pantoya, M., 2004. The effect of size distribution on burn rate in nanocomposite thermites: a probability density function study. *Combustion Theory Modelling*, 8, 555-565.
- [6]-Tillotson, T.M., Gash, A.E., Simpson, R.L., Hrubec, L.W., Satcher Jr., J.H. and Poco, J.F. 2001. Nanostructures energetic materials using sol-gel methodologies. *J. Non-Crystalline Solids*, 285, 338-345.
- [7]-Do, I.P.H., and Benson, D.J. 2001. Micromechanical modeling of shock-induced chemical reactions in heterogeneous multi-material powder mixtures. *Int. J. Plasticity*, 17, 641-668.