

**TITLE:** COMPUTER AIDED MULTI-SCALE DESIGN OF SiC-Si<sub>3</sub>N<sub>4</sub> NANOCERAMIC COMPOSITES FOR HIGH-TEMPERATURE STRUCTURAL APPLICATIONS

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## 1. ABSTRACT

### Program Introduction: Rationale and Objective

It is estimated that by using better and improved high temperature structural materials, the power generation efficiency of the power plants can be increased by 15% resulting in significant cost savings. One such promising material system for future high-temperature structural applications in power plants is Silicon Carbide-Silicon Nitride (SiC-Si<sub>3</sub>N<sub>4</sub>) nanoceramic matrix composites. The proposed research focuses on multiscale simulation-based design of these SiC-Si<sub>3</sub>N<sub>4</sub> nanoceramic matrix composites. There are two primary objectives of the proposed research:

- ✓ **Development of a multiscale simulation tool** and corresponding multiscale analyses of the high-temperature creep and fracture resistance properties of the SiC-Si<sub>3</sub>N<sub>4</sub> nanocomposites at nano-, meso- and continuum length- and timescales; and
- ✓ **Development of a simulation-based robust design optimization methodology** for application to the multiscale simulations to predict the range of the most suitable phase morphologies for the desired high-temperature properties of the SiC-Si<sub>3</sub>N<sub>4</sub> nanocomposites.

The proposed multiscale simulation tool is based on a combination of hybrid molecular dynamics and Monte-Carlo method (HMC), cohesive finite element method (CFEM), and continuum level modeling for characterizing time-dependent material deformation behavior.

### Accomplishments Achieved During the Current Period of Performance

During the current period of performance, January 1, 2007 – March 31, 2008, the HMC method and CFEM methods for the SiC-Si<sub>3</sub>N<sub>4</sub> composites were developed. The continuum level material model for CFEM is incorporated in a 2-D computational material design tool that is being extended to 3-D analyses. A HMC code has been developed and the use of HMC to replace molecular dynamics (MD) as a viable alternative to carry out molecular simulations at higher timescales than currently possible using MD has been established. Young's moduli, defect formation mechanisms, and yield strength values calculated using the HMC and MD always agree with each other very closely which is usually the

main criterions for successful MD simulations. Simulation time analyses show that by using HMC approximately 4 times saving in computational time can be achieved bringing the atomistic analyses closer to the continuum timescales. The CFEM framework was developed for analyzing fracture and creep in digitized micrographs of real experimental SiC-Si<sub>3</sub>N<sub>4</sub> nanocomposite microstructures as well as in hypothetical microstructures with idealized variations in SiC particle volume fractions and the grain boundary (GB) distribution, SiC particle and GB arrangement, and average SiC particle size variation has been developed. Analyses of the damage progression and stress distribution as a function of microstructural morphology indicate that high strength and relatively small sized SiC particles act as stress concentration sites in Si<sub>3</sub>N<sub>4</sub> matrix. Dominant mode of fracture in all microstructures, therefore, is intergranular Si<sub>3</sub>N<sub>4</sub> matrix cracking. The CFEM analyses so far are based on hyper-elastic properties. To include the effect of temperature, a high temperature material model suitable for analyzing fracture and creep as a function of temperature was implemented as a user material interface in finite element code ABAQUS. The model is successful in predicting temperature dependent composite strength relations. The model is now being extended to CFEM based fracture and creep analyses of the nanocomposites. The interfacial properties as a function of temperature are being supplied from atomistic HMC simulations of a combination of configurations of SiC-Si<sub>3</sub>N<sub>4</sub> grain boundaries. A computational material design tool based on variable fidelity model management framework has been developed. In the design tool, complex “high fidelity” FEM analyses are performed only to guide the analytical “low-fidelity” models towards the optimal material design. The tool has been applied to obtain the optimal distribution of the second phase (silicon carbide (SiC) fibers) in the silicon-nitride (Si<sub>3</sub>N<sub>4</sub>) matrix to obtain continuous fiber SiC-Si<sub>3</sub>N<sub>4</sub> ceramic composites (CFCCs) with optimal fracture toughness. Using the variable fidelity design tool in two application studies, one observes a reduction of between 20% and 80% in the design cycle time as compared with a conventional design optimization procedures that exclusively call the FEM. The accuracy of the design is the same as that of the conventional procedures. The design tool is also easily extensible to multi-scale multi-phase material design by using MD based material performance analyses as “high fidelity” analyses that are performed in order to guide “low-fidelity” continuum level numerical tools such as the FEM or finite difference method (FDM) with significant savings in the computational time. Currently design tool incorporates ABAQUS based microstructure models.

### **Plans for the Remaining Period of Performance**

The project is in Phase-II (year-2) now. Remaining months of the phase-II will focus on:

- Use of HMC-CFEM framework to analyze dynamic fracture and creep resistance of SiC-Si<sub>3</sub>N<sub>4</sub> nanocomposites as a function of phase morphology and temperature; and
- Integrate HMC-CFEM framework in the computational design tool for the optimal design of two phase ceramic microstructures and implement a robust optimization approach within the trust region managed interior point optimization framework.

## **2. LIST OF PUBLISHED JOURNAL ARTICLES, COMPLETED PRESENTATIONS AND STUDENTS RECEIVING SUPPORT FROM THE GRANT**

### **International Journal Publications (Accepted or Published)**

1. Mejia-Rodriguez, G., Renaud, J.E., and Tomar V., 2008, A variable fidelity model management framework for designing multiphase materials, *to appear in the ASME Journal of Mechanical Design*
2. Tomar, V., 2008, Analyses of the role of the second phase SiC particles in microstructure dependent fracture resistance variation of SiC-Si<sub>3</sub>N<sub>4</sub> nanocomposites, *Modelling Simul. Mater. Sci. Eng.* 16 (2008) 035001.
3. Tomar, V., 2007, Nanomechanical analyses of nanocrystalline Ni using accelerated molecular timesteps, *Physica Status Solidi-a*, vol. 204 (10), pp. 3340-3348.
4. Tomar, V., 2007, Accelerating the molecular timesteps for nanomechanical simulations: The hybrid Monte Carlo Method, *Journal of Applied Physics*, Vol. 101, pp 103512 (1-9)

### **Students Supported Under this Grant**

- Devendra Dubey, Vikas Samvedi, Charles Penninger, and Gilberto Mejia-Rodriguez (CONACYT Fellowship – grant participant) at Aerospace and Mechanical Engineering, University of Notre Dame