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ANALYSES OF THE EFFECT OF GRAIN BOUNDARIES IN MULTIFUNCTIONALITY OF SIC-SI_3N_4 NANOCOMPOSITES

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ABSTRACT

An advanced nanocomposite microstructure such as that of polycrystalline Silicon Carbide (SiC)-Silicon Nitride (Si_3N_4) nanocomposites contains multiple lengthscales with grain boundary (GB) thickness of the order of 50 nm, SiC particle sizes of the order of 200-300 nm and Si_3N_4 grain sizes of the order of 0.8 to 1.5 μm. Spherical SiC particles are distributed inside the Si_3N_4 matrix in the form of intergranular as well as intragranular dispersions. Because of unique thermal and structural properties, SiC-Si_3N_4 nanocomposites can be used as high temperature structural as well as thermoelectric materials in advanced energy generation systems. In the presented research, combined molecular dynamics (MD) and cohesive finite element method (CFEM) based analyses of dynamic fracture and thermal conductance in bi-modal polycrystalline SiC-Si_3N_4 nanocomposites with an explicit account of multiple length scales associated with GBs, second phase (SiC particles), and the primary phase (Si_3N_4 matrix) are performed.

Classical MD simulations of Si_3N_4+SiC material system require an interatomic potential to describe Si-Si, Si-N, Si-C, N-N, C-C, and N-C interactions. The interatomic potentials for Si_3N_4 material system presented in [1] is used. Different polytypes of SiC exist at ambient pressure, which are differentiated by the stacking sequence of the tetrahedrally bonded Si–C bilayers. Among these polytypes, β-SiC (cubic-SiC) is of much interest for its electronic properties. We use Tersoff potential, [2], for Si and cubic-SiC in the presented research. The framework of MD analyses is based on the work presented in [3]. MD simulations are carried out using a *modified* version of a scalable parallel code, DL_POLY 2.14.

For CFEM analyses bimodal polycrystalline SiC-Si_3N_4 nanocomposite structures are generated with grain sizes of Si_3N_4 in the range of 0.8 to 1.5 μm and SiC particle size varying between 200 nm and 300 nm. The volume fraction of the SiC phase is fixed at 30%. In order to analyze the effect of GBs each sample of SiC-Si_3N_4 nanocomposite has two corresponding meshes: one with finite element (FE) mesh resolving GBs and the other with FE mesh neglecting GBs. Since, a given unique set of phase morphology

defining parameters (such as location of SiC particles, SiC or GB distribution etc.) corresponds to a multiple sets of morphologies, three different random sets of morphologies are used to characterize the material behaviour corresponding to one unique set of phase morphology parameters.

Analyses show that the fracture in the nanocomposites is strongly correlated with the rate of loading, GB distribution, location of SiC particles with respect to GBs and the Si_3N_4 matrix. The effect of GBs becomes stronger with change in temperature (to higher temperatures) with the gap between the fracture strengths of pure intragranular and pure intergranular specimens widening with the increasing temperatures.

The results also reveal that the lattice mismatch and thermal potential differences at the interfaces, and the resulting phonon interface scattering and band structure modifications in super-lattices and nanocomposites can be exploited to reduce phonon heat conduction while maintaining the electron transport. In addition, it is found that the mechanical straining plays an important role in controlling the heat conduction.

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