Multi-scale modeling of irradiated grain boundaries: radiation-induced segregation and corrosion.

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While grain boundaries (GBs) can act as sinks of defects in irradiated materials, much less is known about the effects of radiation on the evolution of the atomic structure of GBs themselves. In addition, in multi-component materials, such as silicon carbide, there can be an unbalanced flux of different species to the GBs, raising questions about potential compositional changes of GBs under irradiation. Such changes could potentially affect the continuing ability of GBs to absorb defects, mechanical properties of the material, and its corrosion resistance.

To address these questions we have developed a multiscale model of defect evolution based on *ab initio* calculations, kinetic Monte Carlo, and rate theory. We have combined these approaches with advanced experimental characterization and applied them to understand defect evolution at interfaces in covalent ceramics. Our models shed light on how tilt and twist grain boundaries accommodate non-equilibrium defects under irradiation. Our models also predict a transition in mechanisms of defect accommodation as a function of temperature, radiation flux, and grain size. In addition, using transmission electron microscopy we found radiation-induced segregation in covalent ceramics. Specifically, using SiC as an example we found that irradiation can either enrich or deplete carbon from grain boundaries, depending on irradiation temperature. The compositional changes also depend on the type of the GB and can be explained using our multiscale models.

In this talk we will also discuss the effects of radiation-induced defects and radiation-induced segregation in GBs on environmental degradation of SiC. We found that in this material incoherent GBs provide a faster oxidation pathway than coherent GBs and the key is a continuous path of oxygen to access highly reactive silicon atoms. All types of point defects were found to accelerate oxidation in crystalline grains of SiC. Although most of these defects accelerate oxidation along GBs as well, surprisingly C antisites were found to suppress oxidation. This trend can be explained by C blocking access of oxygen to highly reactive Si along the GB path.