INTERDISCIPLINARY CENTRE FOR ADVANCED MATERIALS SIMULATION

ICAMS Special Seminar

Prof. Gregory B. Olson

Northwestern University & QuesTek Innovations LLC

Friday, November 18, 1:30 pm. Seminar room UHW 1/127

Integrated Computational Materials Design: From Genome to Flight

The numerical implementation of established materials science principles in the form of purposeful engineering tools has brought a new level of integration of the science and engineering of materials. Building on a system of fundamental databases now known as the Materials Genome, parametric materials design has integrated materials science, applied mechanics and quantum physics within a systems engineering framework to create a first generation of designer "cyberalloys" that have now entered successful commercial applications, and a new enterprise of commercial materials design services has steadily grown over the past decade. The success of computational materials design in the 1990s established a basis for the DARPA-AIM initiative of the 2000s which broadened computational materials engineering to address acceleration of the full materials development and qualification cycle. A new level of science-based AIM modeling accuracy has now been achieved under the ONR/DARPA "D3D" Digital Structure consortium using a suite of advanced 3D tomographic characterization tools to calibrate and validate a set of high fidelity explicit 3D microstructural simulation tools spanning the hierarchy of microstructural scales. Surface thermodynamic “genomic” databases predicted directly from DFT quantum mechanical calculations employing the highly accurate FLAPW method have generated novel “Quantum Steels” completely eliminating intergranular stress corrosion cracking at the highest strength levels, recently demonstrating accelerated flight qualification for aircraft landing gear through application of the integrated computational design + AIM methodology.