INTERDISCIPLINARY CENTRE FOR ADVANCED MATERIALS SIMULATION

ICAMS Special Seminar

Prof. Yunzhi Wang

Department of Materials Science and Engineering
The Ohio State University, USA

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Nanostructure design via non-conventional phase transformation pathways in multi-phase alloys

The key to predicting, and therefore optimizing, properties of materials is the knowledge of the state of microstructure. In multi-phase alloys, precipitate microstructures produced by conventional transformation pathways via nucleation and growth are typically coarse due to limited nucleation events and rapid and unregulated growth after nucleation, limiting severely the utilization of these alloys to their full potentials. In Ti alloys for structural applications, for example, the typical size of α-precipitates in either the colony (slow cooling), basketweave (fast cooling), or equiaxed particle (α/β-processed) morphologies are tens or hundreds of microns. In Ti-Ni alloys for functional and biological applications, the typical domain structures formed are also micron-sized. These coarse domain structures usually have poor balanced mechanical properties for structural applications, and low susceptibility accompanied by large hysteresis for functional applications. This study explores new and non-conventional transformation pathways to develop extremely fine and uniform precipitate microstructures in these alloys, using primarily the phase field method integrated with CALPHAD databases and ab initio calculations. The simulation results are discussed against direct experimental observations of the precipitate microstructures and experimental measurements of the materials responses. The new design strategy may have a profound impact on industrial exploitation of new materials and optimization of existing ones.