INTERDISCIPLINARY CENTRE FOR
ADVANCED MATERIALS SIMULATION

ICAMS Special Seminar

Monday, 17 December, 4:00 p.m.
Room IC 02-718

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Multi-scale modelling of materials processing

Computational materials science offers now tremendous opportunities to formulate next generation process models for metals and alloys which are informed on the atomistic mechanisms of microstructure evolution thereby reducing the number of empirical parameters that are typically used in current process models. The challenges and opportunities of implementing advanced computational materials science tools into process models will be critically reviewed for high-performance steels. Here, the austenite-ferrite transformations are a key metallurgical tool to improve the material properties. Microstructure evolution kinetics depends on interface migration rates that can be significantly affected by alloying elements, e.g. Mn, Mo and Nb in steels. An approach will be illustrated that links atomistic scale models for the solute-interface interaction with phase field modelling to describe the formation of microstructures with complex morphologies. The overall status of the multi-scale modelling approach will be analyzed for intercritical annealing of dual-phase steels and the rapid heat treatment cycles in the heat affected zone of line pipe steels. A critical outlook will be provided to propose future research directions to enhance the computational modelling strategies by truly integrating models across different length and time scales and by extending fundamental model concepts to multi-component systems that are relevant for commercial steel chemistries.