Contribution ID: **55** Type: **not specified**

Advances in phase-field modelling incorporating bulk thermodynamics and interfacial excess quantities

Tuesday 5 November 2019 17:48 (3 minutes)

This work discusses advances in phase-field modelling of multiphase nuclear materials with a focus on incorporating bulk equilibrium thermodynamics and interfacial phenomena. Tools have been developed for the automated construction of explicit multiphase, temperature dependent composite potentials from those of the pure phases obtained from CALPHAD-type databases. The interfacial energy is explicitly controlled and permits consideration of interfacial excess quantities permitting structurally-semicoherent interfaces. This work extends the applicability of bulk thermodynamics to systems dominated by interfacial effects such as nanoscale systems, and kinetically limited, non-equilibrium scenarios. Applications for precipitation of zirconium hydride in fuel cladding, and the evolution of fuel porosity are discussed.

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Session Classification: Poster flash talks