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

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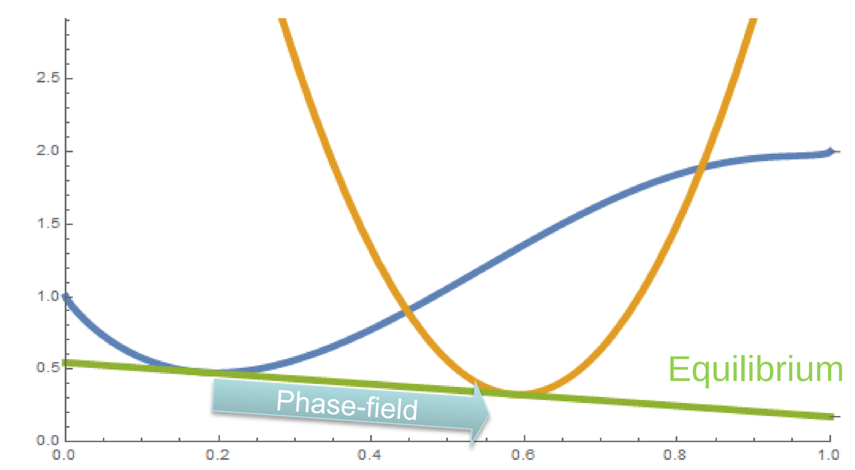
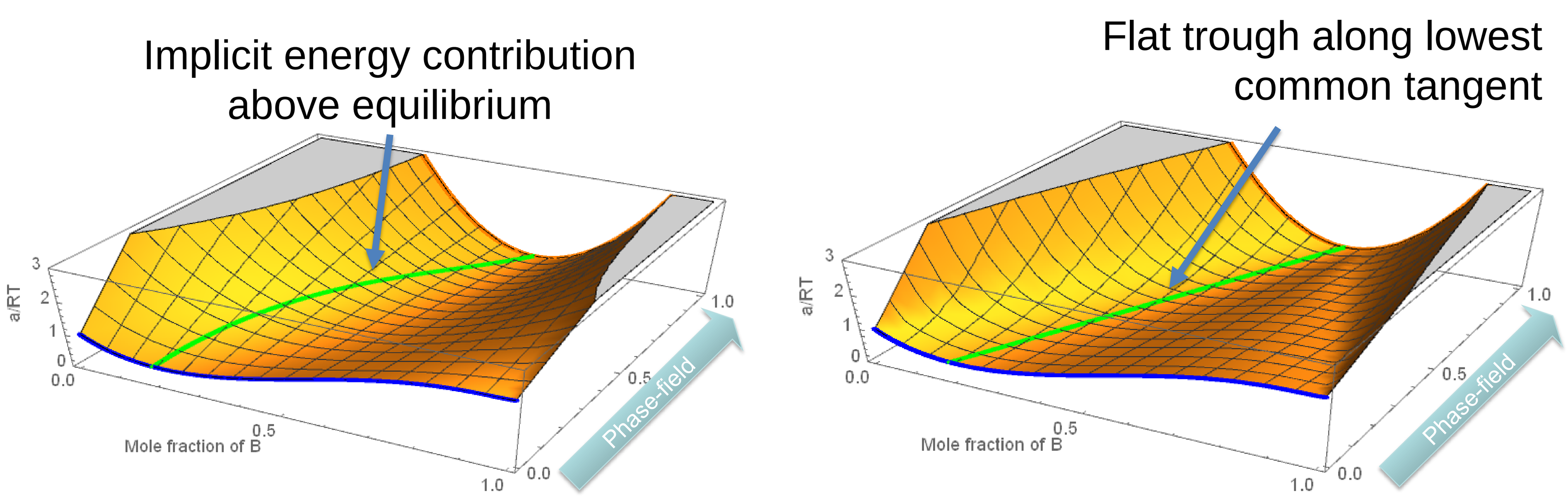
Introduction

Phase-field methods have emerged as powerful tools for capturing interfacial effects and local non-uniformity within multiphysics models with a natural pathway to incorporate bulk thermodynamic potentials. Inclusion of bulk potentials may introduce implicit interfacial energy contributions which may be controlled through the Grand potential formulation of the two-phase composite potential as illustrated below.



Composite potential formed from 2 binary phase potentials showing the appearance of implicit energy contributions.

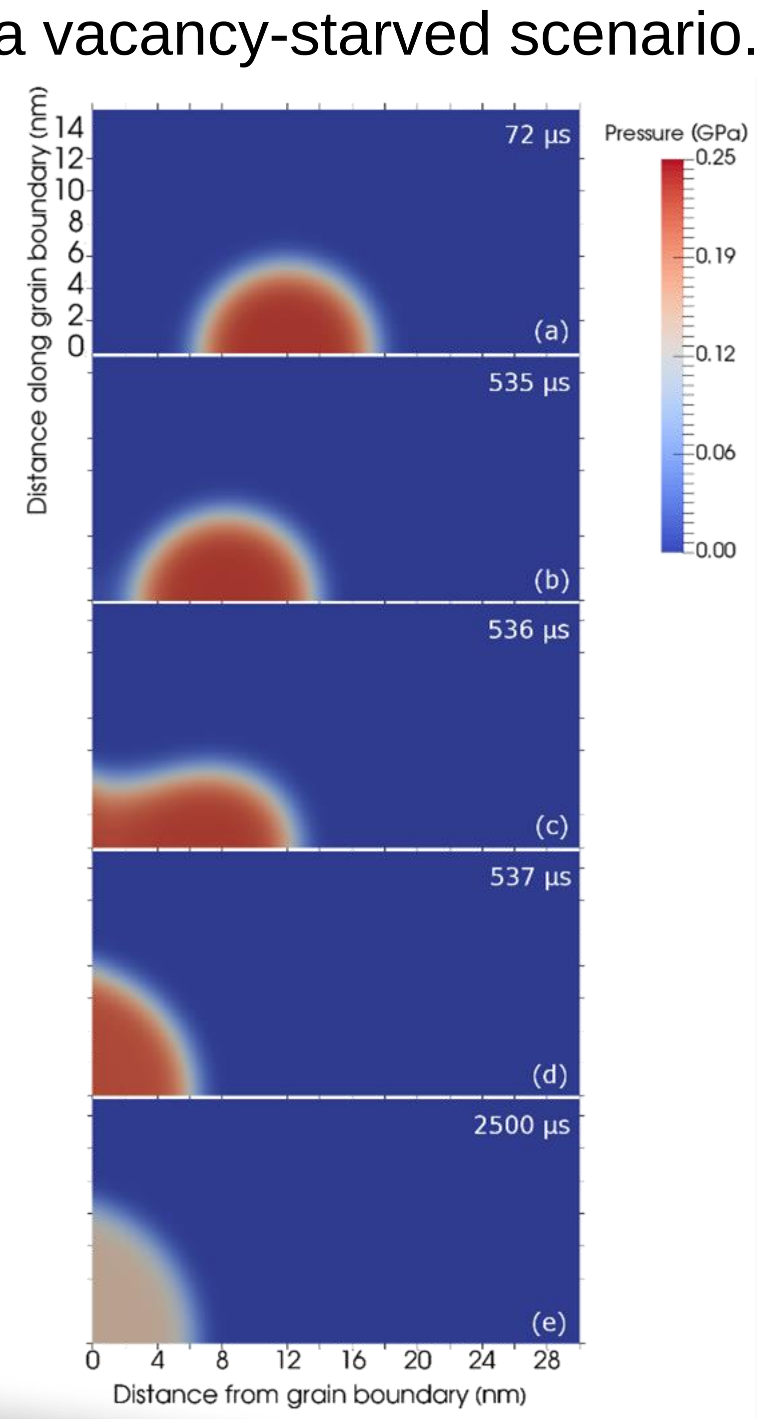


Two examples of the importance of integrating bulk thermodynamic potentials while controlling the interfacial energy are described here.

Vacancy-deficient intragranular bubble

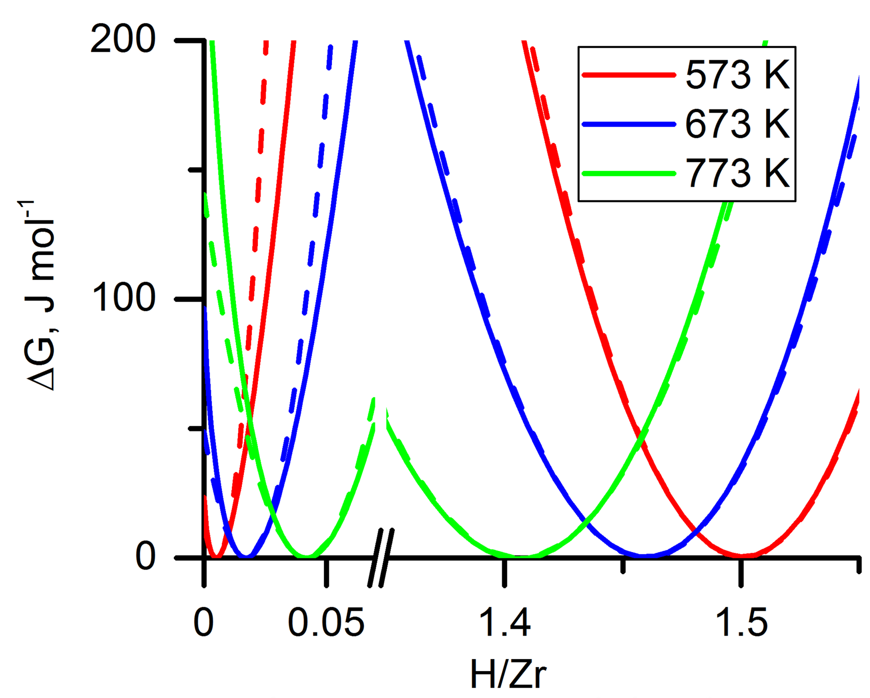
The denuded zone in UO_2 fuel grains is investigated by considering intragranular bubbles in a vacancy-starved scenario.

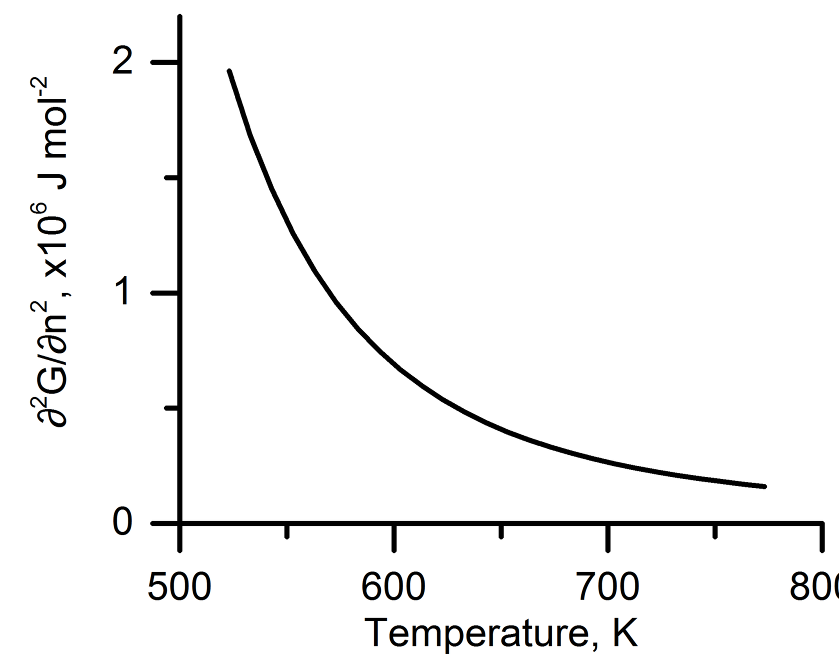
A phase-field model that allows for volumetric dilation and defect migration is coupled with CALPHAD potentials for the gas solubility in the solid matrix. The simulation results (right) shows that the bubble become overpressurised as it is unable to grow due to lack of vacancies. The bubble is attracted to the vacancy-rich grain boundary (the left of the domain) due to the availability of vacancies. Once at the boundary, the bubble grows to relieve its overpressure and assumes a lenticular shape due to interfacial energies.



Zirconium hydride precipitation hysteresis

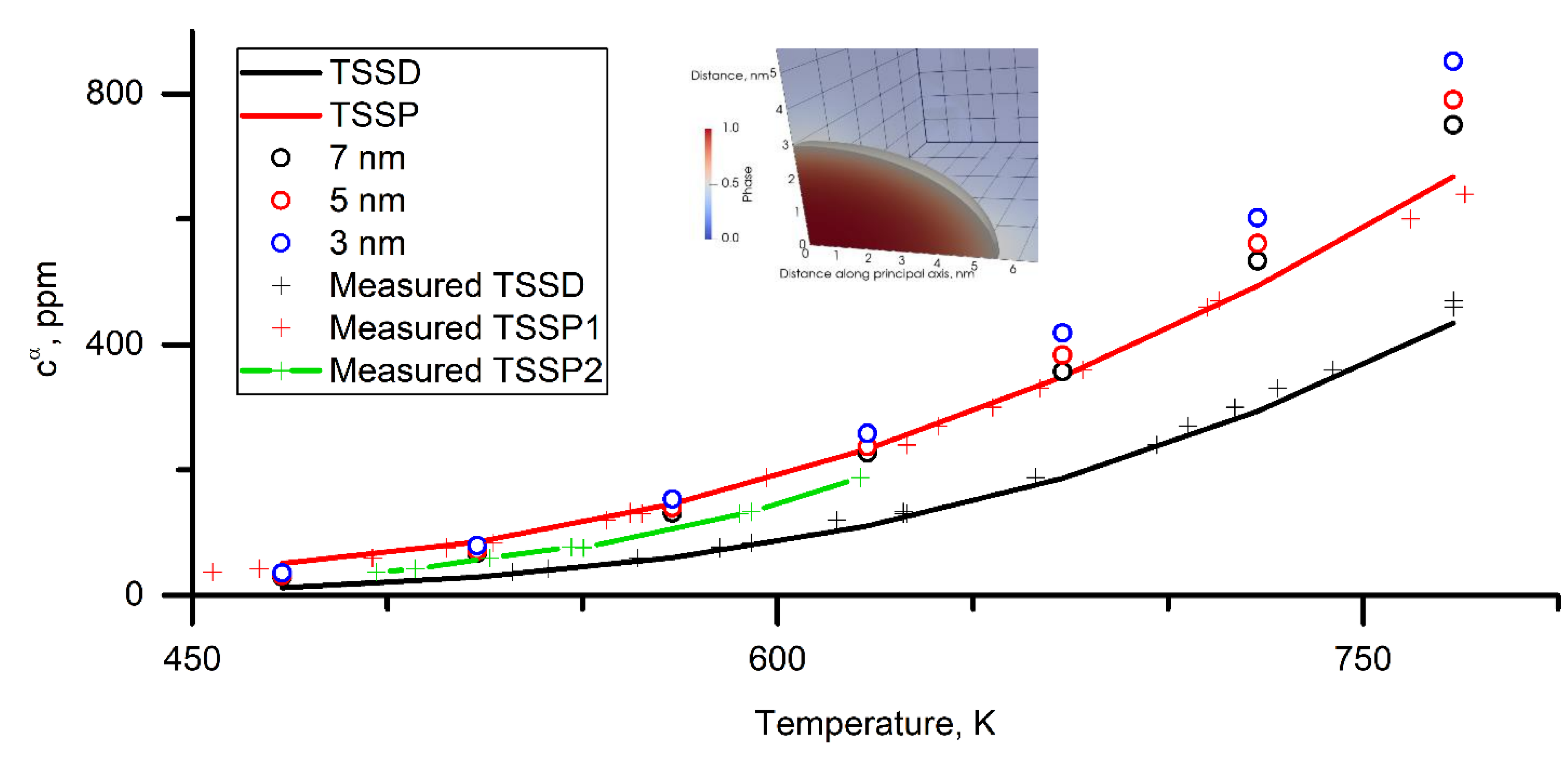
An anisotropic Allen-Cahn phase-field model is applied to the embryotic stage of homogenous δ-hydride nucleation in zirconium to investigate the hysteresis of between the terminal hydrogen solid solubility of dissolution (TSSD) and precipitation (TSSP) in Zr alloys. The thermodynamic potential includes the chemical and elastic state considering an elastically coherent interface and allowing for implicit excess strain energy but eliminating the chemical contribution.





The curvature of the free energy in the α-Zr phase decreases substantially with increasing temperature.

The simulations indicate the widening of the hysteresis gap with increasing temperature results from the change in the curvature of the α-Zr thermodynamic potential which provides the driving force for growth of an embryo. The difference with experimental values may be attributed to homogenous simulated nucleation whereas in practice heterogeneous nucleation aided by residual defects is likely.



The predicted supersaturation - temperature conditions required to grow critical nuclei of 3, 5, and 7 nm semi-major axes compared to TSSP1, TSSP2, and TSSD from complimentary DSC analysis with varying high temperature hold-times.