Metallic fission products phases in nuclear fuels: Thermodynamic modelling of the Mo-Pd-Rh System

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Context

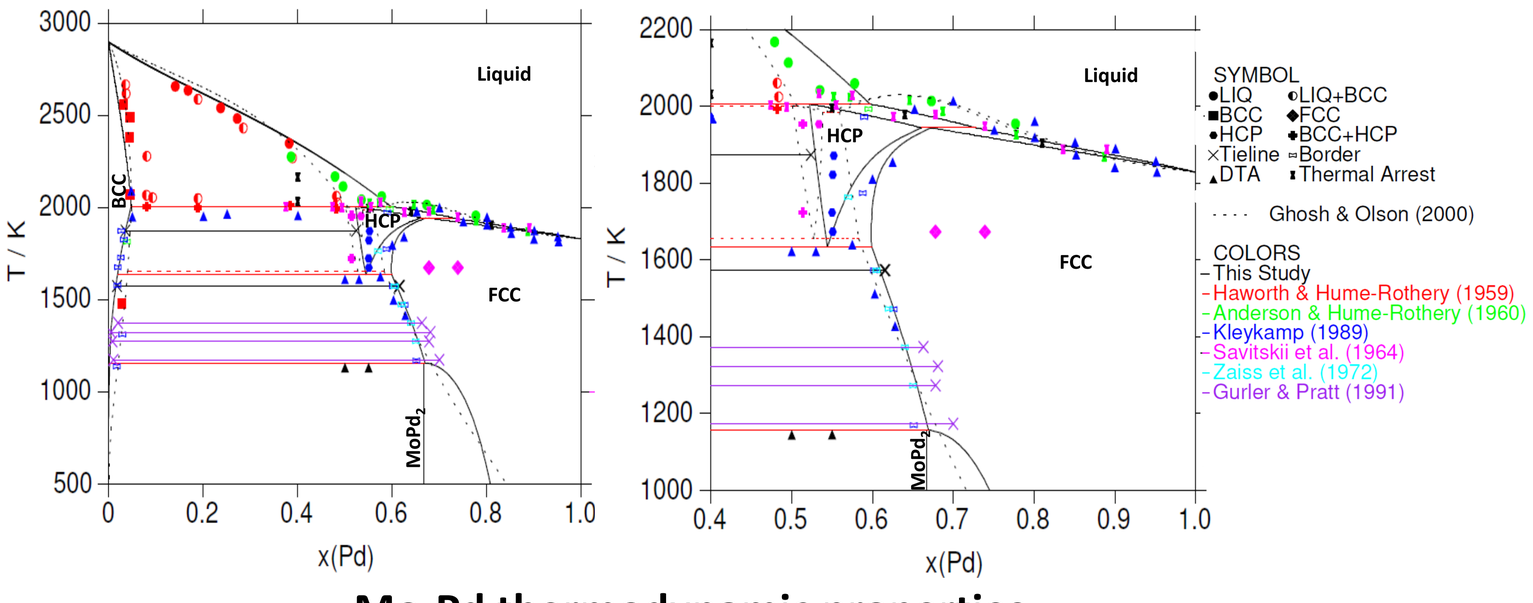
The interest in understanding the thermodynamic behavior of the "white precipitates" Mo-Pd-Rh-Ru-Tc during burn-up of nuclear fuel grew recently. Yet, most of the experimental studies conducted on the Mo-Pd and Mo-Rh binary systems date back to 1960-1990 with new thermodynamic assessment relying mostly on the literature with few to none original data. The new assessments of those systems unveiled inconsistent data between old papers as well as a lack of data at low temperature (under 1250K).

This study is based on a thorough review of the literature and on calculated thermodynamic data to create models that better represent the thermodynamic behavior of both systems. Moreover, experiments are conducted to confirm previous results, to bring new data and to decide between incompatible hypotheses.

The binary systems are the foundations for modeling higher order systems. That's why their assessment should not be neglected.

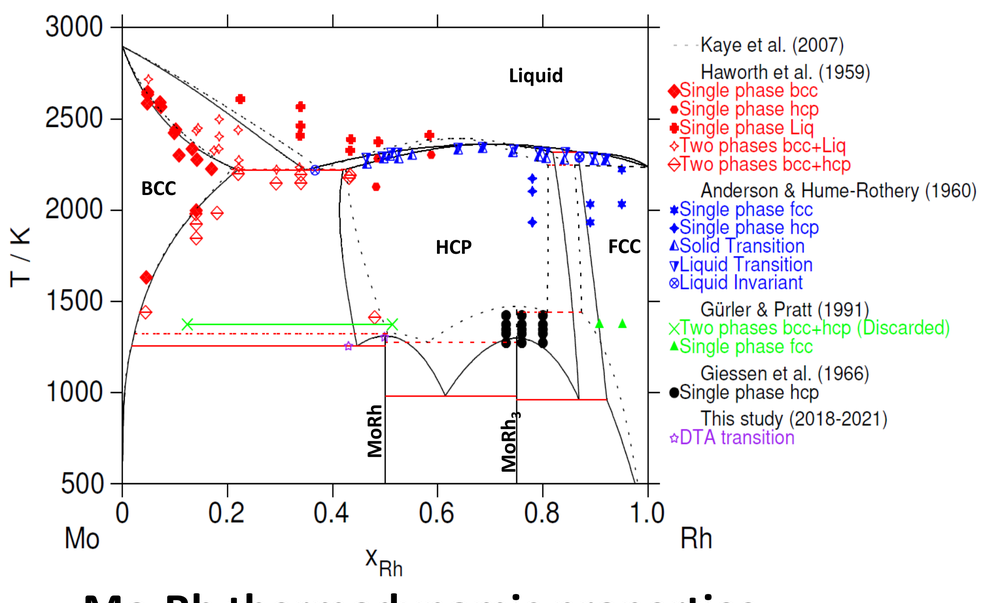
Modeling results (Work in Progress)

Mo-Pd binary



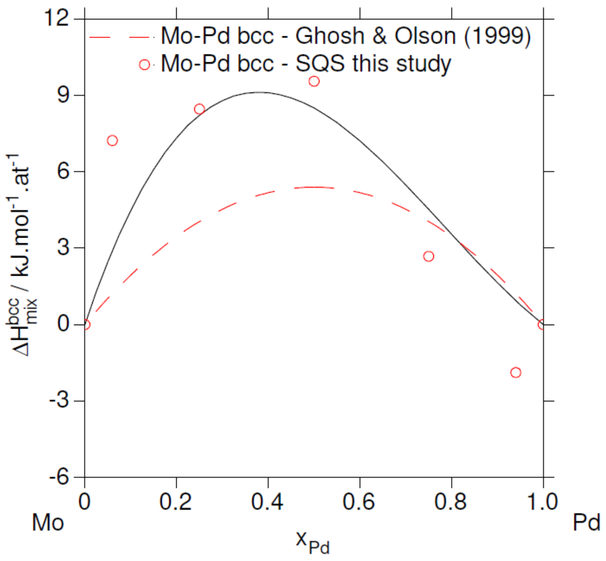
Mo-Pd thermodynamic properties

Mo-Rh binary

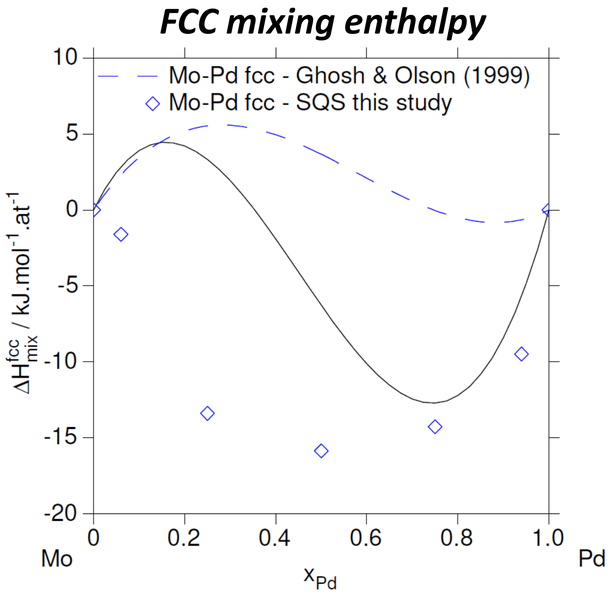


Mo-Rh thermodynamic properties

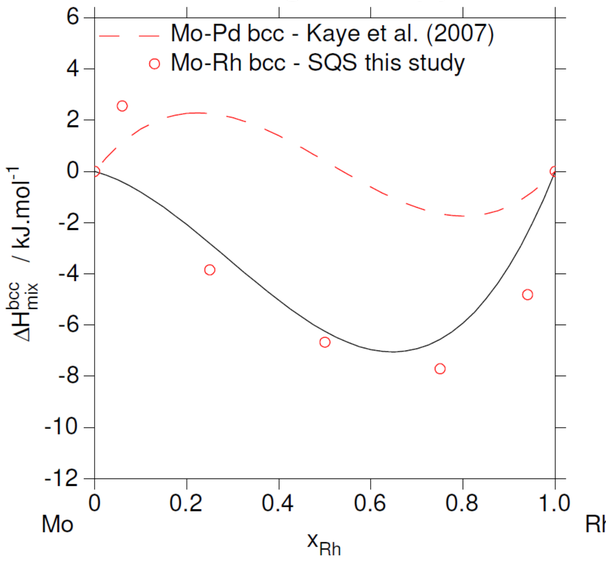
BCC mixing enthalpy



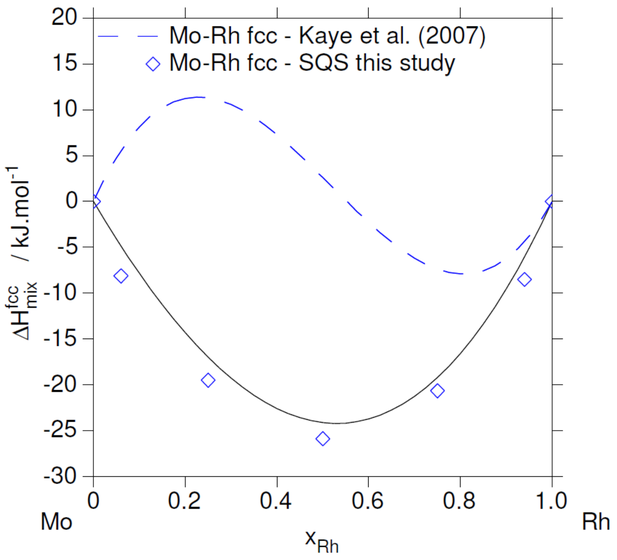
FCC mixing enthalpy



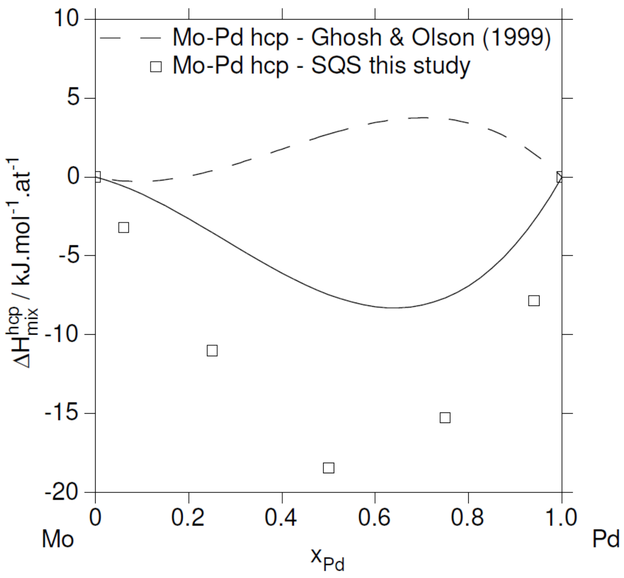
BCC mixing enthalpy



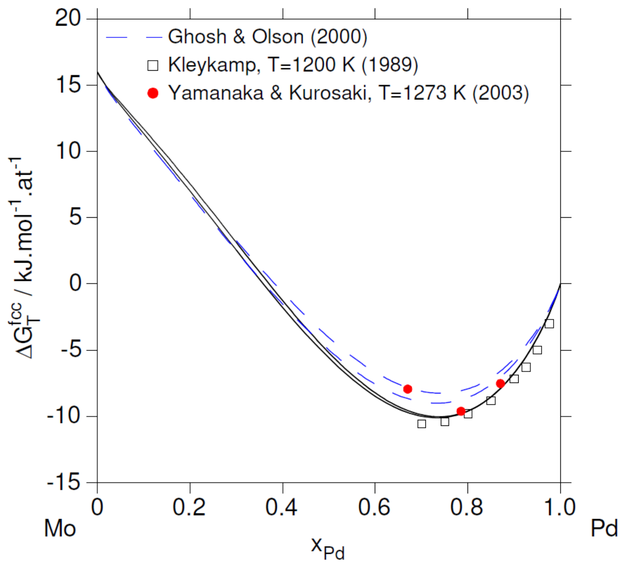
FCC mixing enthalpy



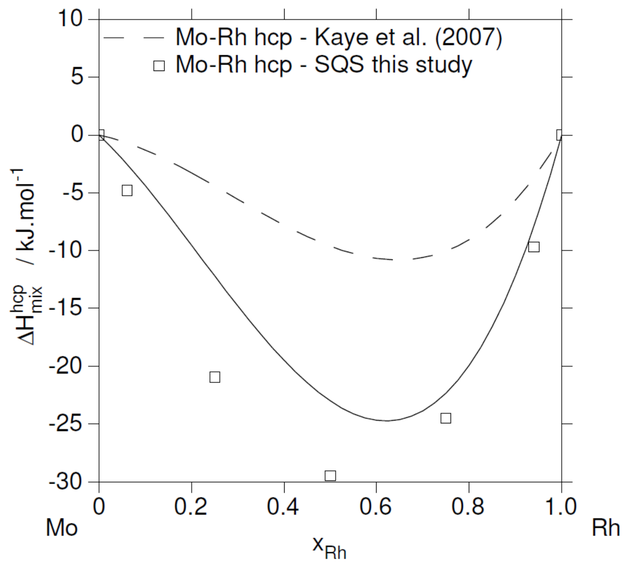
HCP mixing enthalpy



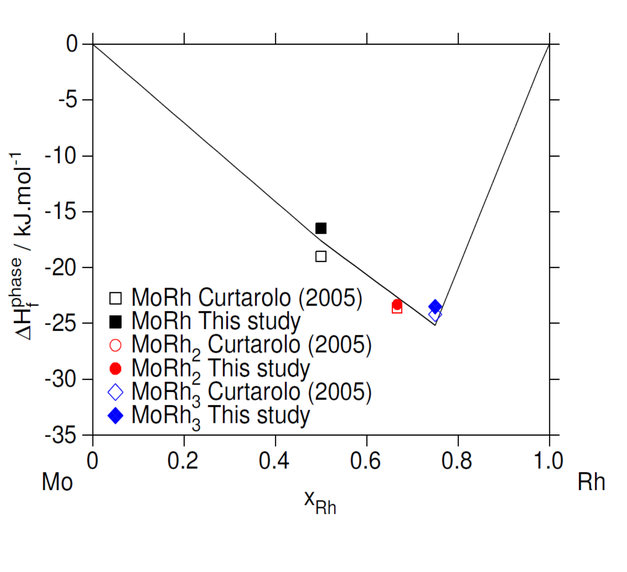
FCC Gibbs energy at 1200 and 1273K



HCP mixing enthalpy



Enthalpy of formation at 298 K



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Conclusion

When compared to the previous models, the ongoing Mo-Pd and Mo-Rh thermodynamic assessment are based on further data coming from DFT+SQS simulations of the solid solutions. With new sets of experimental data, these modeling should give a better representation of the thermodynamic & phase diagram data for the assessment of higher order systems.

On going experiments should soon bring a better understanding of the behavior of Mo-Pd and Mo-Rh alloys at low temperature as well as a better description of the Mo-Pd phase diagram in the FCC-HCP-Liquid area.

Since Mo-Ru binary and Pd-Rh-Ru ternary have already been assessed the next step will focus on Mo systems and Tc binaries and ternaries.