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TUHH Ceramics

INSTITUT FÜR KERAMISCHE HOCHLEISTUNGSWERKSTOFFE

MATERIALWISSENSCHAFTLICHES KOLLOQUIUM

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THE ENIGMATIC AG-PT PHASE DIAGRAM AND YET ANOTHER DERIVATIVE STRUCTURE ALGORITHM

Prof. Dr. Gus HART,

Brigham Young University, Utah, USA

The Ag-Pt phase diagram as published in the most recent phase diagram compilations (Massalski, Pauling File) is entirely speculative below 1000°C. Our recent first principles calculations and cluster expansion-based modelling are largely consistent with the speculations and harbour no big surprises. For example, the phase diagrams and our calculations both suggest a stable $L1_1$ phase at 50 atom %. However, an experimental study published after the compilations supports a significantly different phase diagram. In this new phase diagram, the only stable phases at low temperatures are the elemental fcc Ag and Pt phases and one ordered phase at the unusual concentration of 53±0,5. The experimental study shows that the homogeneity range for the ordered phase is narrow (almost like a line compound), and its X-ray data suggests that the unit cell of this phase contains 32 atoms with a stoichiometry of 15:17. We developed a new derivative structure enumeration algorithm specifically designed for large unit cells with known concentrations. This is necessary because our old algorithm enumerated all concentrations and was therefore limited to smaller unit cells. We have explored, via first-principles, the structural details of this enigmatic phase in the Ag-Pt phase diagram. I will discuss our first-principles results for Ag-Pt, and I will discuss the how the new algorithm is useful for large unit cells when partial structural information is known.

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