

Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

The enigmatic Ag-Pt phase diagram and yet another derivative structure algorithm GUS L.W. HART, LANCE J. NELSON, RODNEY W. FORCADE, Brigham Young University — The Ag-Pt phase diagram as published in the most recent phase diagram compilations (Massalski, Pauling File) is entirely speculative below 1000° C. The phase diagrams and our calculations both suggest a stable L₁ phase at 50 at.-% Pt. 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 at.-% Pt. 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.

Gus L. W. Hart
Brigham Young University

Date submitted: 30 Dec 2010

Electronic form version 1.4