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Thermodynamic properties and equations of state for Ag, Al, Au, Cu and MgO using a lattice vibrational method

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A prerequisite for the determination of pressure in static high pressure measurements, such as in diamond anvil cells is the availability of accurate equations of state for reference materials. These materials serve as luminescence gauges or as X-ray gauges and equations of state for these materials serve as secondary pressure scales. Recently, successful progress has been made in the development of consistency between static, dynamic shock-wave and ultrasonic measurements of equations of state (e.g. Dewaele et al. Phys. Rev. B70, 094112, 2004, Dorogokupets and Oganov, Doklady Earth Sciences, 410, 1091-1095, 2006, Holzapfel, High Pressure Research 30, 372-394, 2010) allowing testing models to arrive at consistent thermodynamic descriptions for X-ray gauges.
Apart from applications of metallic elements in high-pressure work, thermodynamic properties of metallic elements are also of mandatory interest in the field of metallurgy for studying phase equilibria of alloys, kinetics of phase transformation and diffusion related problems, requiring accurate thermodynamic properties in the low pressure regime.

Our aim is to develop a thermodynamic data base for metallic alloy systems containing Ag, Al, Au, Cu, Fe, Ni, Pt, from which volume properties in P-T space can be predicted when it is coupled to vibrational models. This mandates the description of metallic elements as a first step aiming not only at consistency in the pressure scales for the elements, but also at accurate representations of thermodynamic properties in the low pressure regime commonly addressed in metallurgical applications.

In previous works (e.g. Jacobs and de Jong, Geochim. Cosmochim. Acta, 71, 3630-3655, 2007, Jacobs and van den Berg, Phys. Earth Planet. Inter., 186, 36-48, 2011) it was demonstrated that a lattice vibrational framework based on Kieffer's model for the vibrational density of states, is suitable to construct a thermodynamic database for Earth mantle materials. Such a database aims at, when coupled to a thermodynamic computation program, the calculation and prediction of phase equilibria and thermo-physical properties of phase equilibrium assemblages in pressure-temperature-composition space. In Jacobs and van den Berg (2011) the vibrational method, together with a thermodynamic data base, was successfully applied to mantle convection of materials in the Earth.
These works demonstrate that the vibrational method has the advantages of (1) computational speed, (2) coupling or making comparisons with ab initio methods and (3) making reliable extrapolations to extreme conditions.

We present results of thermodynamic analyses, using lattice vibrational methods, of Ag, Al, Au, Cu and MgO covering the pressure and temperature regime of the Earth's interior. We show results on consistency of the pressure scales for these materials using different equations of state, under the constraint that thermodynamic properties in the low-pressure regime are accurately represented.