

APPLICATION OF CALPHAD METHOD TO HIGH PRESSURES

E. Brosh^{1,2}, G. Makov², R.Z. Shneck¹

¹ Department of Materials Engineering, Ben-Gurion University of the Negev,
P.O.Box 653, Beer Sheva, Israel

² NRCN , P.O.Box 9001 Beer-Sheva, Israel

Up to now, attempts to make CALPHAD calculations of high-pressure phase diagrams were largely unsuccessful. The current methods lead to spurious predictions of negative thermal expansion and negative heat capacity at high pressures, without any theoretical justification. The reasons for such failures lie in faulty EOS (Equation Of State) used and in inconsistencies between the EOS and the model used for the ambient-pressure heat capacity. Particularly, it is shown that the Mie-Gruneisen EOS is inconsistent with the widely used SGTE (Scientific Group Thermodata Europe) database. Thus, a combination of the SGTE database with the Mie-Gruneisen EOS, will predict negative heat capacity at high pressure and high temperature. The aforementioned inconsistency is linked to the general problem of describing mechanical instability in CALPHAD. In the present work, we attempt to improve the consistency between caloric and volumetric properties in CALPHAD modelling. Two routes were taken, that lead to the development of 2 new EOS formulations: 1) An explicit Gibbs free energy EOS, that enables the consistent computation of caloric and volumetric properties. 2) A formulation that enables the interpolation of caloric properties between the SGTE database at ambient pressure and the quasi-harmonic model at high pressure. The new formulations were used to calculate the thermodynamic properties and the T-P phase diagrams of Al, Fe, Si, MgO and the Al-Si system.