# Equation of State of NaCl (B1): Thermodynamical approach

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The equation of state (EoS) of NaCl (B1 phase) has been used as the most reliable pressure standard in ultra high-pressure experiments. However any EoS proposed so far for NaCl fails to explain all the necessary constraints of the thermo-physical experimental data. For NaCl EoS, the Debye model and the Mie-Gruneisen EoS with volume dependent Gruneisen parameter (g) are frequently assumed. Spetzler et al. (1972) verified the g(V) hypothesis using ultrasonic data at simultaneous high temperature and high pressure. However we found that Spetzler et al. used inaccurate heat capacity (Cp) data in their analysis. Thus we re-analyze their ultrasonic data with recent Cp data by Archer (1997). The result does not support the g(V) hypothesis. Alternatively, we found that isothermal bulk modulus (Kt) is a function of volume only, or Kt(V).

In the present work, we introduced a new hypothesis of Kt(V). As a result, we can show that the a*Kt (a: thermal expansion coefficient) is a function of temperature only. Combination of these properties and isothermal EoS, we can construct EoS at high pressure and high temperature from experimental data at 1 bar. Although this procedure seems to be limited at 1070 K of melting temperature at 1bar, we can extrapolate the EoS to higher temperature by using the following two equations.

(d a/d P)_V = a(x-Kt)/Kt (eq. 1)

(d x/d P)_V = (Kt*K"+K'(x-Kt)+(d x/d lnV)_P)/Kt (eq. 2)

In these equations, x is defined as (d ln a/d lnV)_P. If we assume that x is a function of volume only at high temperature, equation 2 equals zero. Thus x can be solved as a function of volume from an isothermal EoS. Therefore thermal expansion above melting temperature along an isochore can be estimated from equation 1 from x and a at 1bar and isothermal EoS. This procedure enables us to construct EoS over wide range of temperatures and pressures from limited experimental data.

We apply above procedure to construct EoS from experimental data of thermal expansion and ultrasonic velocities; the 3rd order Birch-Murnaghan EoS is used as an isothermal EoS. The resulted EoS are consistent with experimental constraints, such as thermal expansion at 1bar, ultrasonic velocities, and P-T-V data (Boehler & Kennedy, 1980). The Us-up relation of the shock Hugoniot is also examined, however the present EoS gives faster Us in comparison with the experimental Hugoniot.

References

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