

A.2. Approximations of Potential Functions

It is often found convenient to use simple approximations for the differences between the internal energies of the two phases and also the difference between the Gibbs energies. To demonstrate their accuracy, the approximations are compared to the more accurate equation of state results. It is important to keep in mind that these differences are between values that lie on the equilibrium surfaces. The first useful approximation is for $G_2 - G_1$. Since

$$d(G_2 - G_1) = (V_2 - V_1)dP - (S_2 - S_1)dT ; \quad (\text{A.17})$$

if $V_2 - V_1$ and $S_2 - S_1$ are constant, then

$$G_2 - G_1 = (V_2 - V_1)(P - P^*) - (S_2 - S_1)(T - T^*) , \quad (\text{A.18})$$

the difference between internal energy of the two phases, is

$$E_2 - E_1 = T^*(S_2 - S_1) - P^*(V_2 - V_1) . \quad (\text{A.19})$$

For the approximate calculations, the following values are used: $V_2 - V_1 = -0.00604 \text{ cm}^3/\text{gm}$, $S_2 - S_1 = 3.67 \times 10^{-7} \text{ Mbar cm}^3/\text{gm}$, and $P^* = 0.116 \text{ Mbar}$, $T^* = 332^\circ\text{K}$. Figure A.1 shows the result from the approximate relation for the Gibbs energy differences and those from the more exact equation of state for the mixed phase Hugoniot of iron. The agreement between Eq. (A.18) and the equation of state results is excellent. The approximate

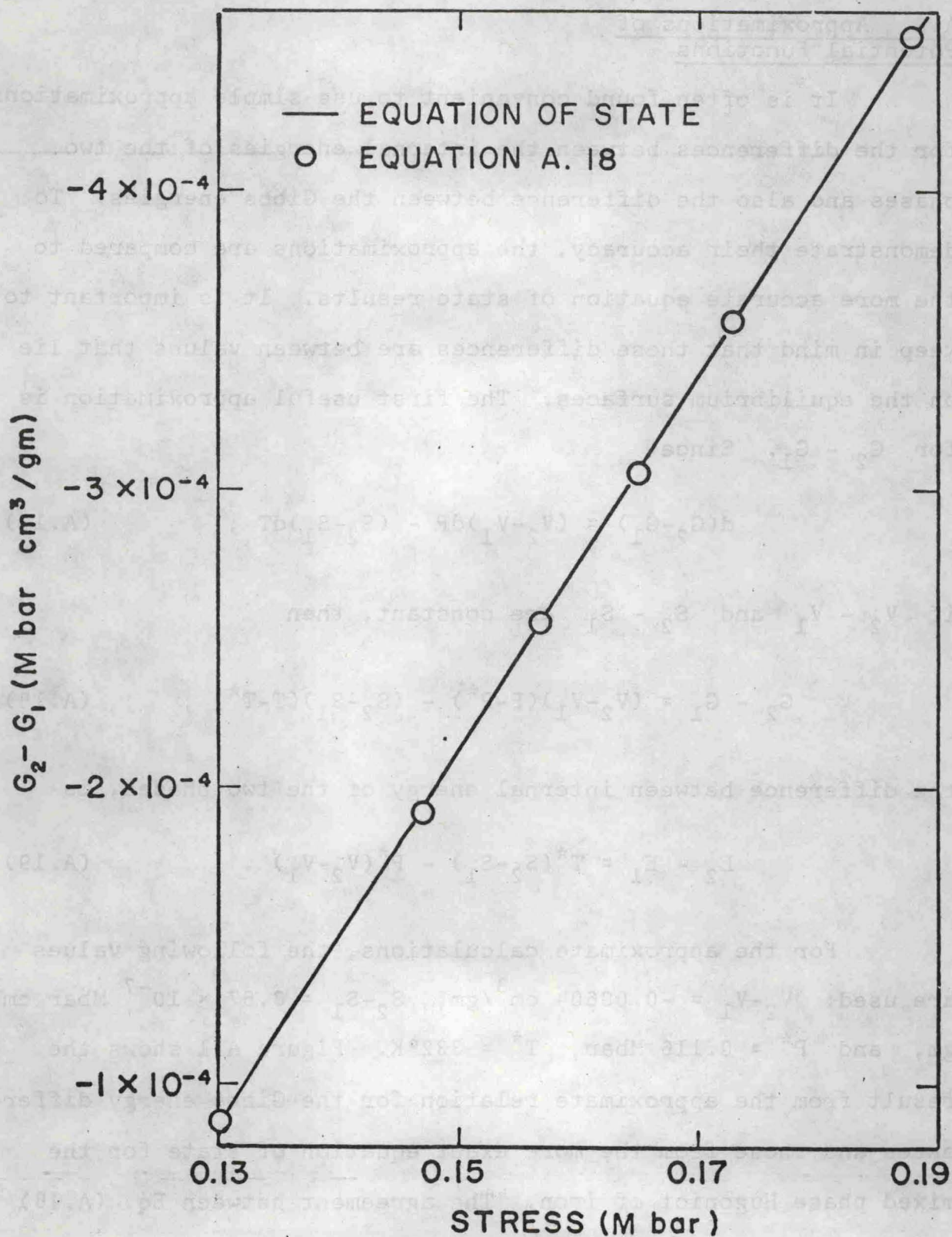


Fig. A.1.--Difference between Gibbs energies of alpha and epsilon iron along the mixed phase Hugoniot.