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Quasistatic Isobaric Heating Test of Three-Phase Equation
of State for Aluminum

Alan M. Winslow

June 1973

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Quasistatic Isobaric Heating Test of Three-Phase Equation
of State for Aluminum

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The aluminum equation of state (EOS 816) used in the LASNEX laser effects calculations was obtained from the three-phase EOS program GRAY.¹ A single table of pressure p (T, V) and a single table of specific energy E (T, V) were made from GRAY calculations to describe the solid, liquid and vapor phases; thus avoiding the necessity of keeping track of the phases in each LASNEX zone. The GRAY results were modified so that, for temperatures $T_V \leq T \leq T_C$ where T_V is the boiling point at atmospheric pressure ($T_V = .2$ ev) and T_C the critical temperature (~ 1 ev), the Van der Waals loops in the pV plane were replaced by horizontal "tie lines": lines of constant pressure along which expansion takes place during change of phase from liquid to vapor. For isotherms with $T < T_V$, however, the pressure p was allowed to become negative as the specific volume V increased, thus introducing tension into the solid and liquid phases. (Fig. 1).

In order to test the accuracy of this EOS, we may perform a simple calculation using only the EOS tables, in which we supply heat Q to a unit mass of aluminum at constant pressure, and observe T and V as functions of Q . For an increment ΔQ of heat absorbed per unit mass we have

$$\left(\frac{\partial E}{\partial T} \right)_V \Delta T + \left[p + \left(\frac{\partial E}{\partial V} \right)_T \right] \Delta V = \Delta Q$$
$$\left(\frac{\partial P}{\partial T} \right)_V \Delta T + \left(\frac{\partial P}{\partial V} \right)_T \Delta V = 0$$
(1)

This system of equations may be solved for ΔT and ΔV using the EOS tables to calculate p and the derivatives of p and E as functions of T^n and V^n , the values of T and V of the beginning of the $(n+1)$ st step. We then advance T and V by means of

$$T^{n+1} = T^n + \Delta T$$

$$V^{n+1} = V^n + \Delta V$$

and repeat (1). For sufficiently small increments ΔQ we should have quasi-static heating, leading to melting and vaporization, at constant pressure.

For initial conditions we set $p = p_0$ and $V = V_0$ (or $T = T_0$) and find the remaining variable by solving $p(T, V_0) = p_0$ or $p(T_0, V) = p_0$ by Newton's method.

The resulting graphs of T vs E and density ρ vs E may be examined for the following properties:

(1) indication of the melting point $T = T_m$ when $E = E_m$, the specific energy to reach melting, and of the vaporization point $T = T_v$ when $E = E_v$, the specific energy to reach vaporization;

(2) constancy of T when $E_m < E < E_m + L_m$ and $E_v < E < E_v + L_v$ where L_m and L_v are the latent heats of melting and vaporization, respectively.

In addition we may observe whether:

(3) the pressure remains constant:

$$p(T, V) = p_0;$$

(4) energy is conserved:

$$E - E_0 + \int p \, dV = Q;$$

(5) the well-known thermodynamic relation

$$p + \frac{\partial E}{\partial V}_T = T \frac{\partial p}{\partial T}_V \quad (2)$$

is satisfied.

We have made this calculation with EOS 816, representing the alloy Al 2024 (4.5% Cu, 1.5% Mg, .6% Mn). We have found experimental values for this alloy only for T_m and E_m . Using Al values for the remaining constants we have:

$$T_m = .078 \text{ ev}, E_m = .51, L_m = .39$$

$$T_v = .219 \text{ (or .233) ev}, E_v = 3.50, L_v = 13.9$$

with E and L in units of 10^{10} erg/g. (For Al, $T_m = .081$ ev and $E_m = .66$.)

For initial values we used $\rho_0 = 2.786 \text{ g/cm}^3$, $T_0 = .0249957$ ev, $p_0 = 10^6 \text{ dyne/cm}^2 = 1 \text{ bar} = .987 \text{ atm}$, $\Delta Q = 10^5 \text{ erg/g}$. The results are shown in Figs. 2-3, from which we observe:

- (a) a break in the slope of T vs E at $E = .6$, representing the melting point;
- (b) a fall in ρ during heating of the liquid reaching $\rho = 2.3 \text{ g/cm}^3$ at $E = 2.4$;
- (c) onset of vaporization at $E = 2.4 - 2.6$, with constant temperature at $T = .216$ ev and rapidly decreasing ρ ;
- (d) the pressure p varies from $p = -11 \text{ b.}$ to $p = +4.4 \text{ b.}$ during melting and heating to vaporization, and remains constant at $p = 4.2 \text{ b.}$ during vaporization.

The calculations also show that E gradually becomes less than Q (the integral $\int p \, dV$ is negligible) the error being 3.4% when $Q = 10$ and 8% when $Q = 15$. Furthermore the ratio of $p + (\partial E / \partial V)_T$ to $T(\partial p / \partial T)_V$ varies from .15 to 6.4.

The expansion of the vapor is shown on a logarithmic scale in Fig. 4. A simple model for this expansion can be obtained by assuming that the mass vaporized is proportional to the fraction $x = (E - E_V)L_V$ for $0 \leq x \leq 1$. This leads to

$$V = V_L + x(V_V - V_L) \quad (3)$$

where V_L , V_V represent the specific volumes of the liquid and vapor respectively. We can solve (3) for ρ_V : V_V^{-1} , and, letting $\rho_L = 2.266 \text{ g/cm}^3 =$ constant, $E_V = 2.0$ we get the curve indicated in Fig. 3. We see that ρ_V rapidly decreases to a value somewhat higher than the ideal gas value $\rho_I = 5.4 \times 10^{-4} \text{ g/cm}^3$ corresponding to the observed temperature and pressure, the departure from ideality no doubt representing attractive forces which tend to increase the density.

If the calculation is repeated with $p_0 = .9 \text{ b.}$, nearly the same results are obtained except that $p = 1.00 \text{ b.}$ and $T = .200 \text{ ev}$ during vaporization. This effect, and also the non-constancy of p , may be attributed to the coarseness of the table which has increments in p of approximately 15 kilobars near $p = 1 \text{ b.}$ Thus the derivatives of p and E may vary considerably along only slightly varying paths in the T, V plane, especially since the EOS interpolation routine does not provide continuity of these derivatives. Because of the steepness of p vs V (see Fig. 1) an impractically large table would be required to reduce the pressure steps significantly. However,

these variations in p , of the order of ± 10 b., are probably not important in our laser effects calculations where rapid heating produces pressures of hundreds of bars.

In conclusion, it appears that EOS 816 gives a fair reproduction of the changes of phase of aluminum during melting and vaporization at $p = 1$ bar. The most significant error is the lack of thermodynamic consistency (Eq. 2). A smoother behavior of $p(T, \rho)$ would also be desirable.

Reference

1. E. B. Royce, "GRAY, A Three-Phase Equation of State for Metals", UCRL-51121 (1971).

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$E(10^{10} \text{ erg/g})$

SQUARE 20 X 20 TO THE INCH AS-0810-GO

Fig. 4

ρ and ρ_v vs E