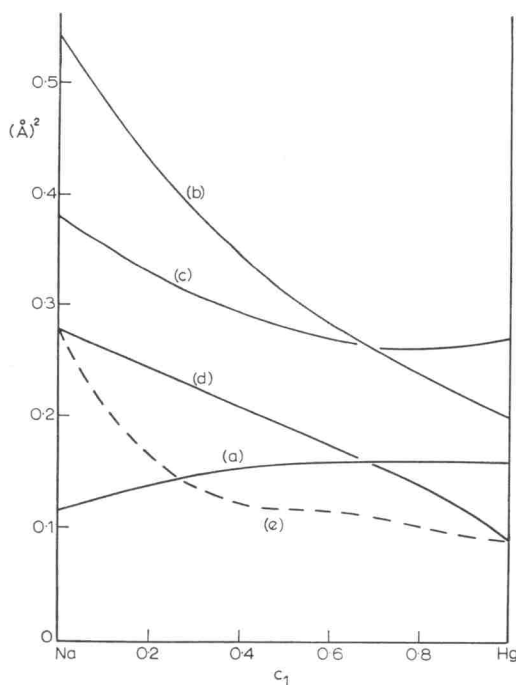


The dielectric constants ϵ' and ϵ and the screening parameter q_S are fully discussed by Faber (1972), who shows how the term $(\epsilon'/\epsilon q_S^2)$ in (7) may be calculated once n is known. This term by itself describes the bulk modulus of the equivalent jellium and includes corrections for correlation and exchange that are well known to be important in this context. The term $-0.08 R_A^2$ may be thought of as an 'umklapp' correction; its evaluation presents no problems. As for R_M^2 , which is a sort of core correction, we might as a first approximation evaluate this by using the values for R_M which have been quoted in various papers by Ashcroft and his colleagues. These are values adjusted, however, to explain properties such as the resistivity which depend upon the behaviour of $u(q)$ at large q ; they do not necessarily describe at all accurately the curvature of $u(q)$ for small q , which is what matters here. The appropriate value of R_M for insertion into (7) may in principle be deduced from any pseudo-potential whose curvature for small q is known, whether or not it is based upon the empty core model, but the tabulated pseudo-potentials which are available in the literature give rather varied results. It therefore seems best to treat R_M as an adjustable parameter.

According to McAlister the isothermal bulk moduli of pure Na and pure Hg at 300°C are 4.3×10^{10} and 18×10^{10} dyne cm⁻² respectively; the corresponding values for K_{int} should be about 4.3×10^{10} and 15×10^{10} . To fit these values with the aid of (7) we require R_M to be 0.73 Å and 0.45 Å for Na and Hg respectively, which appear to be consistent with the pseudo-potentials in current use. The relative magnitude of the three terms in (7) is shown in the figure.



Concentration-dependence in liquid Na-Hg at 300°C of (a) $(\epsilon'/\epsilon q_S^2)_{q \rightarrow 0}$; (b) R_M^2 ; (c) $0.08 R_M^2$; (d) $((\epsilon'/\epsilon q_S^2)_{q \rightarrow 0} + R_M^2 - 0.08 R_A^2)$; (e) $K_{\text{int}}/4\pi(\bar{n}e)^2$.

§ 3. EXTENSION TO ALLOYS

Equation (7) should still be valid for a binary alloy, granted the assumptions listed in § 1 above, provided that $\bar{n}$, $\overline{R_M^2}$ and $\overline{R_A^2}$ are replaced by appropriate mean values, $\bar{n}$, $\overline{R_M^2}$ and $\overline{R_A^2}$. It is not difficult to show (see, for example, the discussion of $w_{\alpha\beta}$ on p. 434 of Faber (1972)) that

$$\overline{R_M^2} = \frac{(c_0 z_0 R_{M,0}^2 + c_1 z_1 R_{M,1}^2)}{c_0 z_0 + c_1 z_1}, \quad \dots \quad (9)$$

where $R_{M,0}$ and $R_{M,1}$ are the core radii for solvent and solute ions respectively, which we may take to be independent of concentration. The umklapp term involves the partial interference functions $a_{00}(q)$, $a_{11}(q)$ and $a_{01}(q)$. For many alloy systems the behaviour of these three functions near their main peaks is likely to be similar to the behaviour of $a(q)$ for a pure liquid. In that case the most plausible interpolation formula for $\overline{R_A^2}$ turns out to be

$$\overline{R_A^2} = \frac{3\Omega}{4\pi} \left[\frac{c_0^2 z_0^2 R_{A,0}^{-1} + 2c_0 c_1 z_0 z_1 (\frac{1}{2}(R_{A,0} + R_{A,1}))^{-1} + c_1^2 z_1^2 R_{A,1}^{-1}}{(c_0 z_0 + c_1 z_1)^2} \right]. \quad (10)$$

Equations (9) and (10) have been used to calculate the concentration-dependence of $\overline{R_M^2}$ and $-0.08\overline{R_A^2}$ in liquid Na-Hg and the results are plotted in the figure. A third curve shows the expected variation of $(\epsilon'/\epsilon q_S^2)_{q \rightarrow 0}$ and a fourth one shows the sum of these three quantities.

It may be seen that the fourth curve is almost a straight line, and it looks as though it would turn out that way for many other systems besides Na-Hg. In that case the theory implies that

$$K_{\text{int}} \cong \bar{n}^2 \left[\frac{c_0 K_{\text{int},0}}{n_0^2} + \frac{c_1 K_{\text{int},1}}{n_1^2} \right], \quad \dots \quad (11)$$

and hence that for dilute alloys

$$\left(\frac{1}{K_{\text{int}}} \frac{dK_{\text{int}}}{dc_1} \right)_{c_1 \rightarrow 0} \cong 2 \left(\frac{z_1 - z_0}{z_0} \right) - 2 \left(\frac{1}{\Omega} \frac{d\Omega}{dc_1} \right)_{c_1 \rightarrow 0} + \left(\frac{\Omega_1^2 z_0^2 K_{\text{int},1}}{\Omega_0^2 z_1^2 K_{\text{int},0}} - 1 \right). \quad (12)$$

To improve upon these simple predictions would require more information about partial structure factors than is yet available.

§ 4. DISCUSSION

A broken curve in the figure shows how $(K_{\text{int}}/4\pi(\bar{n}e)^2)$ varies with concentration for liquid Na-Hg at 300°C according to McAlister. (In deriving K_{int} from McAlister's curve for K_T it has been assumed that $(T/K_T)(\partial K_T/\partial T)_\Omega$ varies with concentration in a linear fashion between the values quoted above for the pure constituents.) The agreement with experiment is far from satisfactory.

The Na-Hg system is not a particularly straightforward one, of course; it is possible that the compound NaHg_2 survives in the liquid phase, and this could affect the compressibility. The disagreement between theory and experiment