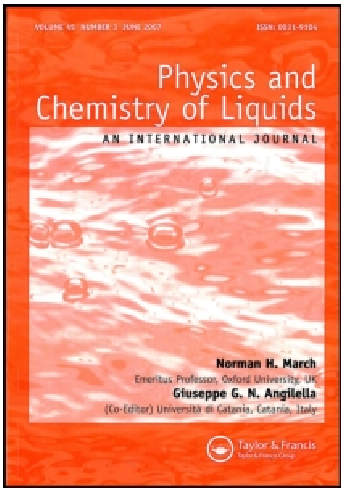

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Correlation Between Potential Well Depth and Melting Temperature of Liquid Metals

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LETTER

Correlation Between Potential Well Depth and Melting Temperature of Liquid Metals

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Characteristic energies of liquid metals obtained from experimental structure factors via a square-well potential are correlated with melting temperature. An approximate linear relationship, $\varepsilon/k_B = 0.246\ T_m$, is proposed and compared with previous correlations reported in the literature.

KEY WORDS: Liquid metals, characteristic energy, melting temperature

The principle of corresponding states has been applied to the viscosity of liquid metals by Chapman[1]. The reduced shear viscosity $\eta^*(V^*, T^*) = \eta\delta^2\mathrm{N}/(\mathrm{MRT})^{1/2}$ was considered to be a function of the reduced volume $V^* = V/N\delta^3$, and reduced temperature $T^* = k_B\mathrm{T}/\varepsilon$. Here, ε is the maximum energy of attraction, i.e., the minimum in the pair potential $\phi(r)$ vs r plot and δ is the collision diameter, the value of r at $\phi(r) = 0$. From experimental ε, δ and η for sodium and potassium[2] and the assumption that all liquid metals obey the same $\phi(r)$, Chapman determined a corresponding states reduced viscosity function plot of $\eta^* V^{*2}$ vs T^{*-1}. Using this plot, together with the assumption that δ was identifiable with Goldschmidt atomic diameters at 0 K, Chapman used experimental coefficients of viscosity to obtain characteristic energies for twenty one metallic liquids. ε/k_B was found to be a linear function of Kelvin melting temperature, viz. $\varepsilon/k_B = 5.20\ T_m$.

Helfand and Rice[3] have extended the principle of corresponding states to the transport properties of fluids obtaining expressions for the reduced shear viscosity $\eta^*(T^*, P^*) = \eta\delta^2/(M\varepsilon)^{1/2}$ and reduced self diffusion coefficient $D^*(T^*, P^*) = (D/\delta)(M/\varepsilon)^{1/2}$. Pasternak[4] has applied these expressions to an analysis of liquid metal η and δ data. When the reduced pressure $P^* = P\delta^3/\varepsilon$ can be neglected, $\eta^* V^*/D^* = \upsilon/D$, where υ is the kinematic viscosity. Plots of υ/D vs T^{*-1} could be superimposed by adopting suitable ε for each metal relative to $\varepsilon/k_B = 1970$ K for sodium[2]. For ten liquid metals an approximately linear function between ε/k_B and T_m was observed, viz. $\varepsilon/k_B = 5.20\ T_m$ together with almost linear relations between $\eta^* V^{*2/3}$ or $D^*/V^{*1/3}$ and T^{*-1}. Similar analyses have been presented by Wittenberg and Dewitt[5] and by Waseda and Ohtami[6]. By multiplication of the reduce viscosity by the reduced volume raised to the power required to cancel δ from Chapman's reduced viscosity function, i.e. $\eta^* V^{*2/3}$, Pasternak[4] avoided the necessity to specify explicit values of δ.

Collings[7] has questioned the suitability of the relative ε values obtained by Chapman and by Pasternak in the light of more recent X-ray and neutron diffraction data for liquid sodium and potassium[8]. It was suggested, that application of the Born-Green and Percus-Yevick theories give more appropriate ε values. While ε obtained from the latter theory are less than those obtained from the former theory, they are similar in magnitude and between 1/5 to 1/2 of those obtained by Chapman. Collings suggests also that the linear correlation of ε/k_B and T_m is more appropriately represented by $\varepsilon/k_B = 1.32\ T_m$.

By considering a square-well attractive tail as a perturbation on the hard sphere pair potential, Gopala Rao and Joardar[9] have derived an equation of state through

Table 1 ε/k_B values for liquid metals (K)

Metal	T_m (*K*)	*Chapman*	*Pasternak*	*BG*[a]	*PY*[b]	*SW*[c]	*MSW*[d]
Na	371	1970	1970	582	442	111.6^{12}	116.5^{11}
K	336.65	1760	—	578	360	96.14^{12}	148.7^{11}
Li	452.15	2350	2380	454	450	—	—
Mg	922	4300	—	—	—	127.82^{14}	224.9^{10}
Al	933.25	4250	—	879	735	160^{19}	169.8^{10}
Ca	1120	5250	—	—	—	—	—
Fe	1809	10900	—	—	—	425.67^{13}	269.2^{10}
Co	1768	9550	—	—	—	403.64^{13}	—
Ni	1726	9750	—	—	—	531.29^{13}	814.5^{10}
Cu	1357.6	6600	6440	—	—	300^{15}	260.9^{10}
Zn	692.655	4700	3770	—	—	—	—
Rb	312.64	1600	—	424	361	96.14^{12}	—
Ag	1234	6400	6250	—	—	500^{15}	290.4^{10}
Cd	594.26	3300	—	—	—	282.79^{14}	—
In	429.78	2500	2230	—	—	173.76^{16}	—
Sn	505.06	2650	2510	—	—	—	—
Cs	301.55	1550	—	694	230	109.5^{12}	—
Au	1337.58	6750	—	—	—	600^{15}	—
Hg	234.28	1250	1200	649	192	100^{19}	—
Pb	600.6	2800	2750	1180	879	70^{18}	203.6^{10}
Ga	302.8	—	1730	—	—	218^{18}	—
Tl	576.6	—	—	—	—	157.97^{16}	—
Pt	2042	—	—	—	—	332.28^{17}	—
Pd	1825	—	—	—	—	245.49^{17}	—
Bi	544.52	—	—	—	—	252.1^{21}	—
La	1193	—	—	—	—	—	505.4^{11}

[a] Born-Green
[b] Percus-Yevick
[c] Square-Well
[d] Modified (Improved) Square-Well

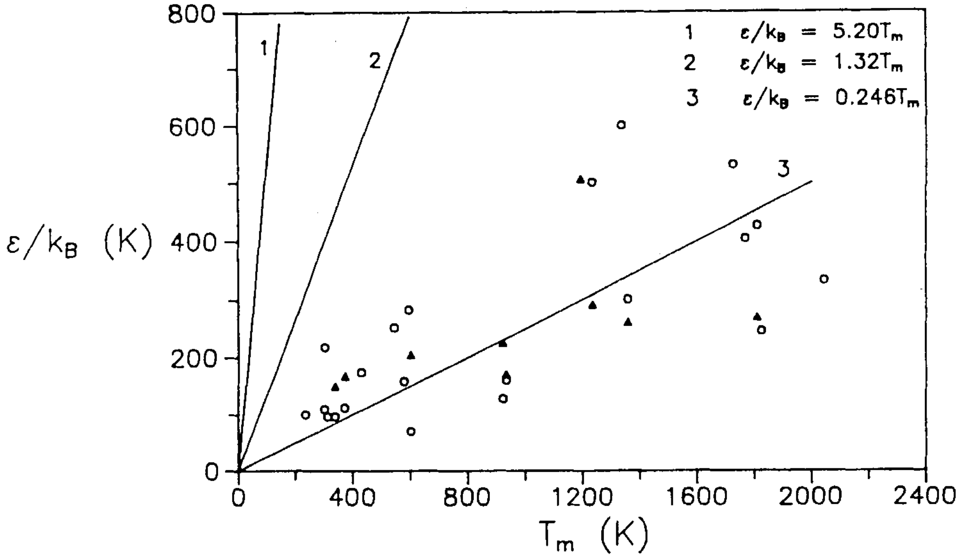

Figure 1 Correlation of ε/k_B and melting temperature for liquid metals ○ square-well potential, ▲ modified square-well potential.

the direct correlation function in the long wavelength limit viz. $PV/RT = (1 + y + y^2)/(1 - y)^3 - 4y\varepsilon(\lambda^3 - 1)/k_BT$. Here $y = \pi\sigma^3\rho/6$ denotes the packing fraction of atoms with diameter σ, ε and λ are the depth and width of the square-well potential, and $\rho = N/V$ is the number density. All other symbols have their usual connotations. ε and λ can be obtained by fitting experimental structure factors S(Q) at the first peak position. A modified square-well potential[10,11] with an attractive part inside the hard core softens the steep repulsive core and gives better agreement for S(Q) within the low Q region.

Gopala Rao *et al.*[10–19] reported characteristic energies of several liquid metals obtained via the square-well and modified square-well, hard sphere pair potentials from experimental structure factors. These are reported in Table 1, together with ε/k_B values obtained by other workers. Melting temperatures given in the table were taken from the compilation by Hultgren *et al.*[20] It is apparent from Table 1 that $(\varepsilon/k_B)_{SW}$ values are substantially smaller than those of other estimates. In Figure 1, $(\varepsilon/k_B)_{SW}$ is linearly correlated with T_m for twenty one metallic elements. Least squares analysis of the data yields $\varepsilon/k_B = 0.246\ T_m$. Characteristic energies are thence easily estimated from melting temperatures for other metals. For comparison purposes, Figure 1 includes the lines for previous ε/k_B vs. T_m correlations and ε/k_B values obtained using a modified square-well potential.

Silbert and Young[21] and Bretonnet *et al.*[22] have fitted a hard sphere repulsive ledge-type potential to a number of liquid metals. These calculations suggest that a repulsive potential ($\varepsilon > 0$) may be more appropriate to metals characterised by shoulders (Ga and Bi) on the high-angle side of the first peak of S(Q). Bretonnet *et* *al.* [22] suggest that a ledge-type potential is also appropriate for Pb, Mg, Hg, Na and to a lesser extent Ag. The suggested correlation of ε/k_B and T_m reported in this communication is restricted to hard sphere square-well fluids.

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