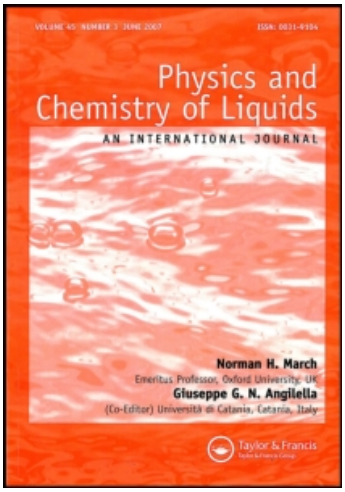

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Temperature dependence of sound velocity in liquid metals

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Temperature dependence of sound velocity in liquid metals

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In this article, we report comparisons between theoretical and experimental values of the velocity of sound and its temperature coefficient at the melting temperature for 41 liquid metals using a number of model theories.

Keywords: Sound velocity; Liquid metals; Temperature coefficient

1. Introduction

Except in a few anomalous metals like Si, Ge, Sb, Te, Ce and Pu, the velocity of sound c decreases slowly with increasing temperature T in liquid metals. The logarithmic temperature derivative $(\partial \ln c/\partial \ln T)_P$ is typically between -0.1 and -0.3 at the melting temperature T_m. As a consequence, accurate values of the temperature coefficient of sound velocity $(\partial c/\partial T))_P$ require measurement of sound velocities over extended temperature ranges. The wide variation in reported values of $(\partial c/\partial T)_P$ for a given liquid metal is probably attributable to sound velocity measurements carried out over limited temperature ranges. The purpose of this article is to investigate the temperature dependence of the velocity of sound in liquid metals in terms of a number of model theories and to compare $(\partial c/\partial T)_P$ values obtained with critically appraised literature values.

2. Model theories

2.1. *Tsagareishvili's approach*

Tsagareishvili [1] has developed a quasi-thermodynamic approach, which allows approximate integration of exact thermodynamic equations. Here, $(\partial c/\partial T)_P$ may be

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expressed by logarithmic differentiation of the exact relation between the adiabatic bulk modulus B_S, sound velocity c and density ρ

$$B_S = \frac{1}{\rho c^2} \tag{1}$$

$$\left(\frac{\partial \ln c}{\partial T}\right)_P = \frac{1}{2}\left(\frac{\partial \ln B_S}{\partial T} - \frac{\partial \ln \rho}{\partial T}\right)_P \tag{2}$$

Using the substitutions [2],

$$\left(\frac{\partial \ln B_S}{\partial T}\right)_P = -2\alpha\Gamma \tag{3}$$

$$\left(\frac{\partial \ln \rho}{\partial T}\right)_P = -\alpha \tag{4}$$

equation (2) may be written as

$$\left(\frac{\partial c}{\partial T}\right)_P = -\alpha c\left(\Gamma - \frac{1}{2}\right) \tag{5}$$

In equations (5) and (6), α is the expansivity, C_P the isobaric heat capacity and Γ the Grűneisen parameter defined by

$$\Gamma = \frac{\alpha c^2}{C_P} \tag{6}$$

Using equations (5) and (6) we calculate $(\partial c/\partial T)_P$ at the melting temperature for the 41 liquid metals for which sound velocity versus temperature data are available in the literature. The results are summarised in table 1.

2.2. *Gitis and Mikhailov's approach*

From statistical mechanical considerations, Gitis and Mikhailov [3] have expressed the velocity of sound in terms of the cohesive energy U and atomic weight M as

$$c = \left(\frac{2U}{M}\right)^{1/2} \tag{7}$$

The cohesive energy may be related to the atomic volume V, pair distribution function $g(r)$, pair potential $\phi(r)$ and Avogadro number N_o by

$$U = \frac{2\pi N_o^2}{V}\int_o^\infty g(r)\varphi(r)r^2 \mathrm{d}r \tag{8}$$

The enthalpy of vapourisation $\Delta_l^g H$ is also given by

$$\begin{aligned}\Delta_l^g H &= RT - \frac{2\pi N_o^2}{V}\int_o^\infty g(r)\varphi(r)r^2\,\mathrm{d}r = RT - U \\ &\approx U \quad \text{since } RT \ll |U|\end{aligned} \tag{9}$$

Table 1. Temperature coefficients of sound velocity $(\partial c/\partial T)_P$ calculated from model theories for liquid metals at the melting temperature.

Metal	$-(\partial c/\partial T)_P$	$-(\partial c/\partial T)_P$	$-(\partial c/\partial T)_P$	$-(\partial c/\partial T)_P$	$-(\partial c/\partial T)_P$	$-(\partial c/\partial T)_P$
	$m\,s^{-1}\,K^{-1}$ [a]From ρ_e	$m\,s^{-1}\,K^{-1}$ [b]From $\Delta_l^g H$	$m\,s^{-1}\,K^{-1}$ [c]From α,c,C_P	$m\,s^{-1}\,K^{-1}$ [d]From ρ	$m\,s^{-1}\,K^{-1}$ [e]From ρ, z_Γ	$m\,s^{-1}\,K^{-1}$ Experimental
Li	–	0.66	0.63	1.70	2.51	0.60
Be	–	0.39	0.60	1.03	1.49	0.72
Na	4.80	0.46	0.35	1.26	2.55	0.44
Mg	0.13	0.41	1.07	0.91	1.72	0.58
Al	1.11	0.24	1.99	0.98	1.37	0.48
Si	2.55	0.18	0.89			−0.93
K	4.45	0.39	0.41	0.84	1.46	0.59
Ca	–	0.26	0.21	0.57	0.75	0.49
Mn	–	0.28	0.26	0.88	1.24	0.15–0.59
Fe	0.33	0.24	0.14	0.72	1.17	0.50
Co	0.52	0.18	1.19	0.71	1.20	0.46
Ni	0.24	0.20	0.46	0.76	1.39	0.39
Cu	0.59	0.14	0.87	0.55	0.78	0.49
Zn	–	0.25	0.81	0.47	0.89	0.34
Ga	0.99	0.15	0.46	0.25	0.39	0.26
Ge	–	0.11	0.28	–	–	−3.50
Se	–	0.09	0.06	0.62	1.47	1.07
Rb	2.32	0.25	0.27	0.49	0.84	0.34
Sr	–	0.22	0.14	0.44	0.83	0.31
Mo	−0.01	0.12	1.26	0.34	0.58	0.47
Ag	0.63	0.14	0.73	0.39	0.56	0.39
Cd	–	0.19	0.81	0.35	0.54	0.39
In	0.71	0.14	0.55	0.26	0.41	0.29
Sn	0.56	0.11	0.50	0.23	0.49	0.28
Sb	0.16	0.13	0.20	–	–	−0.23
Te	–	0.14	−0.02	–	–	−0.97
Cs	–	0.23	0.22	0.49	0.86	0.30
Ba	–	0.21	0.0002	0.27	0.57	0.18
La	0.15	0.10	0.04	0.20	0.35	0.08
Ce	0.09	0.11	−0.01	–	–	−0.18
Pr	0.15	0.14	0.03	0.47	0.84	0.08
Yb	0.06	0.17	0.17	0.43	1.30	0.20
Ta	0.03	0.08	0.74	0.32	0.56	0.26
W	–	0.06	0.71	0.31	0.56	0.47
Pt	0.02	0.08	0.52	0.48	0.86	0.24
Au	0.49	0.08	0.91	0.29	0.40	0.57
Hg	–	0.18	0.61	0.21	0.42	0.48
Tl	0.26	0.11	0.40	0.23	0.46	0.23
Pb	0.39	0.11	0.48	0.22	0.32	0.28
Bi	0.29	0.11	0.36	0.21	0.31	0.04
Pu	–	0.10	−0.03	–	–	−0.08

[a] Gitis and Mikhailov's approach (electrical resistivities); [b]Gitis and Mikhailov (vapourisation enthalpies); [c]Tsagareishvili's approach; [d]Modified Rosenfeld's approach; [e]Modified Ascarelli's approach.

Thus, equation (7) becomes

$$c = \left(\frac{2\Delta_l^g H}{M}\right)^{1/2} \tag{10}$$

and the temperature coefficient of sound velocity based on equation (10) is

$$(\partial c/\partial T)_p = -cC_P/2\Delta_l^g H \tag{11}$$

Using equations (10) and (11), we calculate sound velocities and temperature coefficients $(\partial c/\partial T)_P$ at the melting temperature for the liquid metals listed in tables 1 and 2. The results are summarised in tables 1 and 2. Vapourisation enthalpies and isobaric heat capacities used in the calculations were taken from the compilation by Barin [4]. Values for selenium and tellurium are based on the hexamer and dimer, respectively, as the principal vapour species. Velocities of sound estimated from vapourisation enthalpies are compared with measured values in figure 1.

2.3. *Gitis and Mikkhailov's approach [5]*

The temperature dependence of the electrical conductivity σ is determined by the relation

$$\sigma = z\theta^2 \tag{12}$$

where z is the number of valence electrons per atom and θ the Debye temperature. Differentiation of equation (12) gives

$$\frac{1}{\sigma}\left(\frac{\partial\sigma}{\partial T}\right)_P = \frac{1}{z}\left(\frac{\partial z}{\partial T}\right)_p + \frac{2}{\theta}\left(\frac{\partial\theta}{\partial T}\right)_p \tag{13}$$

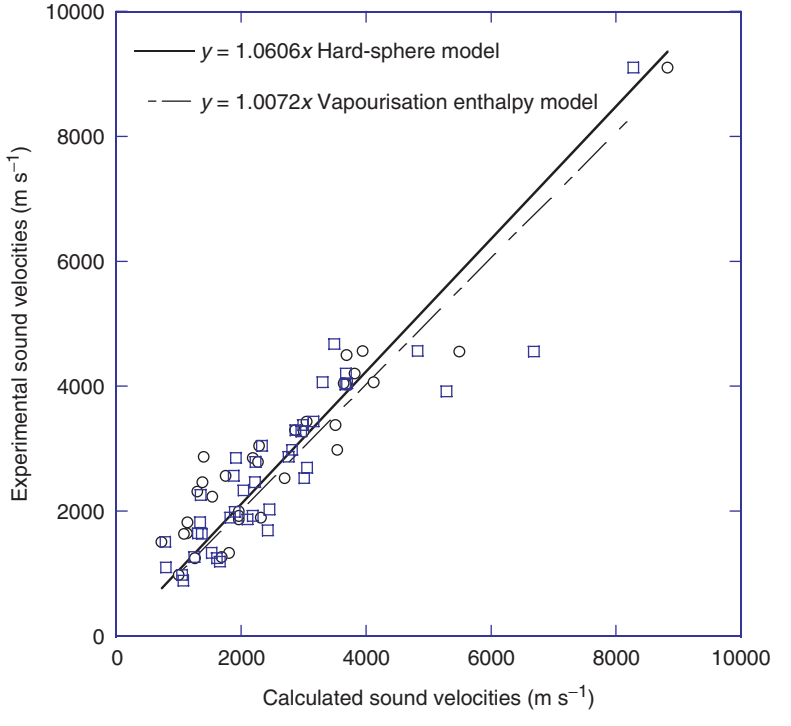

Figure 1. Comparison between theoretical and experimental velocities of sound in liquid metals at the melting temperature.

Expressing the Debye temperature in terms of the velocity of sound, viz.,

$$c = \left(\frac{k_B}{h}\right)\left(\frac{4\pi}{3N_o}\right)^{1/3}\left(\frac{M}{\rho}\right)^{1/3}\theta \tag{14}$$

where k_B and h are Boltzmann's and Planck's constants, respectively. Differentiation of equation (14) gives

$$\frac{1}{c}\left(\frac{\partial c}{\partial T}\right)_P = -\frac{1}{3\rho}\left(\frac{\partial \rho}{\partial T}\right)_P + \frac{1}{\theta}\left(\frac{\partial \theta}{\partial T}\right)_P \tag{15}$$

Equation (15) may be substituted in equation (13) to give:

$$\left(\frac{\partial c}{\partial T}\right)_P = \frac{c}{2\sigma}\left(\frac{\partial \sigma}{\partial T}\right)_P + \frac{\alpha c}{3} - \frac{c}{2z}\left(\frac{\partial z}{\partial T}\right)_P \tag{16}$$

Regarding the electron concentration as constant and since the electrical resistivity ρ_e is the reciprocal of the electrical conductivity, equation (16) may be expressed as

$$\left(\frac{\partial c}{\partial T}\right)_P = -\frac{c}{2\rho e}\left(\frac{\partial \rho e}{\partial T}\right)_P + \frac{\alpha c}{3} \tag{17}$$

Using equation (17), we calculate $(\partial c/\partial T)_P$ for 26 liquid metals at the melting temperature using data for ρ_e and $(\partial \rho_e/\partial T)_P$ from Iida and Guthrie [6] together with expansivities from the compilation by Crawley [7]. The results are summarised in table 1.

2.4. *Rosenfeld's approach (hard-sphere model)*

Following Rosenfeld [8], the velocity of sound may be expressed as

$$c = S(\eta)\left(\frac{k_B T}{M}\right)^{1/2} \tag{18}$$

where

$$S(\eta) = \left(p(\eta) + \eta p'(\eta) + \frac{2}{3}p(\eta)^2\right)^{1/2} \tag{19}$$

and $p(\eta)$ is the Carnahan–Starling compressibility factor, which is expressed in terms of the packing factor η of the hard-sphere fluid and is defined by

$$p(\eta) = \frac{1 + \eta + \eta^2 - \eta^2}{(1-\eta)^3} \tag{20}$$

and where the first derivative of the of the compressibility factor is

$$p'(\eta) = \left(\frac{\partial p(\eta)}{\partial \eta}\right) = \frac{2(2 + 2\eta - \eta^2)}{(1-\eta)^4} \tag{21}$$

Table 2. Comparison between theoretical and experimental velocity of sound of liquid metals at the melting temperature.

	[a]c m s^{-1}	[b]c m s^{-1}	[c]c m s^{-1}	[d]c m s^{-1}	[e]c m s^{-1}	[f]c m s^{-1}	c_{expt} m s^{-1}
Li	6690	5484	5492	5128	4892	6898	4554
Na	3009	2725	2699	2451	2335	3501	2526
K	2101	1990	1966	1720	1673	2694	1876
Rb	1613	1297	1260	1183	1156	1821	1251
Cs	1058	1022	1004	860	838	1442	983
Be	8282	8923	8825	10928	9988	10579	9104
Mg	3304	4177	4126	4600	4050	4945	4065
Ca	2818	3573	3533	4356	3147	4202	2978
Sr	1827	2348	2316	2061	1947	2663	1902
Ba	1531	1832	1807	1499	1379	1751	1331
Al	4826	3990	3944	5934	4450	4843	4561
Si	5291	–	–	6662	4922	–	3920
Mn	2997	3565	3508	3536	3200	3593	3381
Fe	3679	3861	3812	4555	3896	4118	4200
Co	3669	3715	3674	4287	3687	4097	4031
Ni	3692	3679	3638	3703	3507	4367	4047
Cu	3158	3136	3050	3022	3101	3644	3440
Zn	1920	2208	2182	2736	1563	2829	2850
Ga	2764	1413	1398	2672	1662	2259	2873
Ge	3056	2770	–	3365	2454	2833	2693
Se	793	1695	–	2508	1743	3031	1100
Mo	3495	3728	3685	4804	3610	3769	4502
Ag	2229	2294	2268	2157	2236	2962	2790
Cd	1357	1559	1542	1862	1573	2135	2237
In	2038	1312	1297	1693	1255	1985	2320
Sn	2222	1399	1383	1862	1299	1866	2464
Sb	1900	1848	–	2409	1654	2214	1988
Te	1072	1614	–	2509	1181	1775	889
La	2456	1988	1967	1958	1731	2407	2002
Ce	2427	1875	–	1705	1499	2433	1693
Pr	2190	1983	1960	2153	1799	2142	1925
Yb	1248	1708	1688	1672	1431	2004	1274
Ta	2876	2891	2859	3492	2958	3314	3303
W	2966	3035	3001	3957	3219	3519	3277
Pt	2338	2196	2283	2629	2234	2428	3053
Au	1880	1768	1748	1759	1858	2264	2568
Hg	785	733	724	1245	858	1124	1511
Tl	1306	1140	1127	1524	1140	1601	1650
Pb	1348	1155	1142	1569	1103	1597	1821
Bi	1372	1095	1082	1989	1142	1468	1640
Pu	1659	–	–	–	–	–	1195

[a]Gitis and Mikhailov approach (vapourisation enthalpies); [b]Rosenfeld's approach; [c]Modified Rosenfeld's approach; [d]Ascarelli's approach; [e]Ascarelli's approach using z_f; [f]Modified Ascarelli's approach.

The packing fraction η is defined in terms of the hard-sphere diameter a, viz.,

$$\eta = \frac{\pi a^3 N_o \rho}{6M} \tag{22}$$

Hard-sphere diameters at the melting temperature conform closely with the relationship $a^3/V_m = (1.484 \pm 0.025) \times 10^{-24}$, equivalent to a packing fraction $\eta = 0.468$. Using equations (18)–(22), we calculate velocities of sound at the melting temperature, as shown in table 2.

2.5. *Modified Rosenfeld's approach*

Taking account of the temperature dependence of the hard-sphere diameter, Yokoyama [9] has modified equation (19) as

$$S(\eta) = \left(p(\eta) + \eta p'(\eta) + \frac{2}{3}\left(p(\eta) + 3\eta p'(\eta)\left(\frac{\partial \ln\, a}{\partial \ln\, T}\right)_V\right)^2\right)^{1/2} \tag{23}$$

The logarithmic temperature coefficient of the hard-sphere diameter may be derived from the empirical expression of Protopapas *et al.* [10],

$$a = a_o\left(1 - 0.112\left(\frac{T}{T_m}\right)^{1/2}\right) \tag{24}$$

in which

$$a_o = 1.0788\left(\frac{N_o \rho_m}{M}\right)^{-1/3} \tag{25}$$

and

$$\left(\frac{\partial \ln\, a}{\partial \ln\, T}\right)_V = -0.056\left(\frac{a_o}{a}\right)\left(\frac{T}{T_m}\right)^{1/2} \tag{26}$$

The a_o values determined using equation (25) are equivalent to a value of $\eta = 0.468$ as applicable at the melting temperature, where ρ_m is the liquid density at T_m. Equation (24) allows hard-sphere diameters to be determined at a given temperature, the resultant values together with melt densities and equation (22) being used to determine η at these temperatures. Equation (26) is used together with the calculated a and a_o values to obtain$(\partial \ln a/\partial \ln T)_V$.$\eta$ values are used together with equations (20) and (21) to determine $p(\eta)$ and $p'(\eta)$, respectively. $S(\eta)$ may now be determined from equation (23) and thence c using equation (18). Excluding the anomalous metals, we calculate velocities of sound values as a function of temperature for 35 metallic liquids and thence $(\partial c/\partial T)_P$ at the respective melting temperatures. The results are summarised in tables 1 and 2. Velocities of sound calculated from the modified Rosenfeld hard-sphere model are compared with measured values in figure 1. For purposes of clarity, the individual elements are not labelled in figure 1.

2.6. *Ascarelli's approach*

Ascarelli [11] has shown that a simple model of hard spheres immersed in a uniform (without gradients) background potential is able to describe the velocity of sound and its temperature dependence in liquid metals of widely differing atomic masses, densities and melting temperatures. Using the hard-sphere equation of state of Reiss *et al.* [12], together with an assumed packing fraction of 0.45 as applicable to all metals at their melting point and a constant value of $\gamma = 1.15$, Ascarelli's expression for the velocity of sound is

$$c = \left\{\frac{\gamma k_B T}{M}\left[\frac{(1+2\eta)^2}{(1-\eta)^4} + \frac{2zE_F}{3k_B T} - \left(\frac{4AT_m}{3T}\right)\left(\frac{V_m}{V}\right)^{1/3}\right]\right\}^{1/2} \tag{27}$$

where $\gamma = C_P/C_V$ is the ratio of isobaric to isochoric heat capacities, E_F the Fermi energy and V_m/V the ratio of molar volumes at the melting temperature T_m and temperature T, respectively. The coefficient A is defined by

$$A = 10 + (2zE_F/5k_BT) \tag{28}$$

The temperature dependence of the packing fraction was determined in terms of the packing fraction at constant volume η_V using

$$\eta = \frac{\eta_V V_m}{V} \tag{29}$$

where

$$\left(\frac{(1+\eta v+\eta v^2)}{(1-\eta v)^2}\right) = 3.7 + (6.3T/T_m) \tag{30}$$

Using equations (27)–(30), Ascarelli determined $(\partial c/\partial T)_P$ accounting for the role of electrons and reported $(\partial c/\partial T)_P$ for a number of elements, Rb (−0.3), Zn (−0.2), In (−0.14) and Sn (−0.15), all in units of $m\,s^{-1}\,K^{-1}$. At the melting temperature equation (27) becomes

$$c = \gamma k_B T_m/M[27 + (2zE_F/15k_BT_m)] \tag{31}$$

Using equation (31) together with Fermi energies and γ values from the literature, we calculate velocities of sound at the melting temperature using both chemical and effective valences. The results are summarised in table 2.

2.7. *Modified Ascarelli's approach*

Yokoyama [13,14] has also accounted for the influence of electrons on the velocity of sound in metallic liquids using modifications of the Ascarelli theory. Essentially these include use of the Protopapas procedure for estimating the temperature dependence of the hard-sphere diameter, use of the more robust Carnahan–Starling equation of state, a value of $\eta = 0.463$ as applicable at T_m, and a nonconstant γ. Additionally, a more comprehensive account is taken of the uniform background potential. The velocity of sound is given by

$$\frac{c^2}{(k_BT/M)} = \left(\frac{1}{k_BT}\right)\left[-0.031\frac{z}{3} - 4\left(\frac{0.916z^{4/3} + 1.8z^2B_H}{9a'}\right) + \frac{22.1z^{5/3}}{9a'^2}\right] + S(\eta)^2 \tag{32}$$

In equation (32), the Wigner–Seitz radius is defined by $a' = (3M/4\pi N_o\rho)^{1/3}$ and the term B_H denotes the electrostatic energy of the point-ion model. Following Yokoyama [14] the explicit expression for B_H in terms of, a'_m,the Wigner–Seitz radius at the melting temperature is

$$B_H = \frac{a'^{\,7}_m}{6}\left[\frac{0.031z}{a'_m} + \left(\frac{0.916z^{4/4} + 1.8z^2}{a'^{\,2}_m}\right) - \frac{4.42z^{5/3}}{a'^{\,3}_m} - \frac{p(\eta)k_BT}{a'_m}\right] \tag{33}$$

Application of equations (32) and (33) requires a knowledge of the valence of the liquid metal. In this work we employ the effective valence z_Γ as determined from the one-component plasma model of the liquid state (OCP). The OCP model is defined in

terms of a system of point-like ions each carrying a charge ze moving in a uniform background potential and having the same number density, ionic mass and temperature as a real fluid. The OCP is characterised by a plasma parameter $\Gamma' = (z_\Gamma e)^2/a' k_B T$, where e is the electronic charge. Γ' values and hence effective valences may be obtained either from diffraction measurements where the value of Γ' is selected so as to well fit the first peak of the experimental structure factors [15] or by fitting the entropy of the OCP system to the observed entropy [16]. In this work we employ the latter method for 37 liquid metals. Measured entropies and melting temperatures were taken from the compilation by Barin [4]. Electronic contributions to the entropy were calculated using Fermi energies from the literature [17,18]. Where appropriate, magnetic contributions to the entropy were considered following Harder and Young [19]. In this work, we use $S(\eta)$ as determined from the modified Rosenfeld approach together with equations (32) and (33) to calculate velocities of sound and their temperature dependence for the nonanomalous metals. The results are summarised in tables 1 and 2.

3. Results and discussion

Calculation of $(\partial c/\partial T)_P$ using the approach suggested by D. S. Tsagareishvili and G. V. Tsagareishvili amounts to the determination of the difference between the terms $\alpha^2 c^3/C_P$ and $\alpha c/2$. The former term having the larger absolute magnitude in the majority of cases and including terms raised to high powers suggests an inherent sensitivity of theoretical $(\partial c/\partial T)_P$ to errors in the measured values of α and c. In nearly half of the elements considered, this approach overestimates $(\partial c/\partial T)_P$ as compared to measured values. $(\partial c/\partial T)_P$ for the alkali metals are in reasonable accord with measurement and the approach correctly predicts a positive (although small) temperature coefficient for Te, Ce and Pu. In the majority of cases, $(\partial c/\partial T)_P$ calculated from vapourisation enthalpies tend to underestimate this quantity when compared with measured values. $(\partial c/\partial T)_P$ values estimated for the alkali and alkali earth elements using vapourisation enthalpies however, may be regarded as reasonable. Sound velocities at the melting temperature estimated from vapourisation enthalpies on the one hand and from density data using the modified Rosenfeld hard-sphere model on the other hand are compared with measured values in figure 1. It is apparent that sound velocities estimated from the former data result in better estimates than those predicted from density data. $(\partial c/\partial T)_P$ estimated from electrical resistivity and expansivity data tend to overestimate $(\partial c/\partial T)_P$ as compared to measured values. Such overestimation is markedly the case for the alkali metals Na, K and Rb. In nearly half of the elements examined, the modified Rosenfeld's approach overestimates $(\partial c/\partial T)_P$, as is readily apparent in the case of the alkali and alkali earth metals. For all the elements examined in the present study, the hard-sphere approach results in $(\partial c/\partial T)_P$ values that decrease progressively with increasing temperature. $(\partial c/\partial T)_P$ values reported in table 1 are those at the respective melting temperatures. For the liquid alkali metals, accurate sound velocities over extended temperature ranges are available and these indicate that $(\partial c/\partial T)_P$ increases progressively with increasing temperature [20, 21]. $(\partial c/\partial T)_P$ estimated from the modified Ascarelli's approach, i.e., accounting for the role of electrons consistently overestimates the temperature coefficient of the velocity of sound as compared with measured values. Comparison of calculated and measured melting temperature sound velocities of the alkali and alkali earth metals indicates that when

account is taken of electronic effects, a significant overestimation occurs. Excluding electronic effects the hard-sphere model with allowance for the temperature dependence of the hard-sphere diameter gives a better description of the melting point sound velocities of these two groups of metals. For the liquid transition metals, on the other hand, the effects caused by accounting for electronic effects are small, typically increasing sound velocity values by ~12%. In the context of accounting for the effects of electrons on calculated sound velocities, the difficulty of assigning effective valences to the transition metals is all important.

4. Conclusions

Temperature coefficients of sound velocities $(\partial c/\partial T)_P$ have been calculated from a number of model theories. At present, none of those examined may be considered to adequately represent measured $(\partial c/\partial T)_P$ values. Simple procedures using vaporisation enthalpies yield better estimates of sound velocities at the melting point than those obtained from the more involved hard-sphere approach.

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