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A new point-ion pseudizing potential for s–p bonded metals*

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Abstract. We have developed a new point-ion pseudizing potential appropriate for the s–p bonded metals. The electron–ion contribution to the effective potential has been calculated self-consistently. The essential feature of this description is the occurrence of the true field rather than a coulombic form in the pre-asymptotic region. The orthogonalizing contributions that arise from repulsive s scattering and attractive p scattering are calculated in terms of delta functions of strengths suitable for achieving the necessary s and p pseudizations respectively. The new potential is successfully applied to calculate a number of solid and liquid state properties of certain s–p bonded systems.

1. Introduction

It is now nearly three decades in which the pseudopotential theory has been a formidable tool in the investigation of a variety of metallic properties. For many simple metallic systems some specific forms of pseudopotentials [1] have proved to be decisive in calculating only a very few properties. At a later stage there has been indeed a significant advance in developing broad-based model potentials which essentially embrace the refined and more general aspects of the underlying microscopic properties in a self-consistent fashion [2–4]. These aspects consider a global appeal including non-locality, energy dependence and other relevant refinements in the electron–ion interaction. In other words, these attempts have been pushing forward the frontiers of the pseudopotential framework to match those generated by the non-perturbative approach [5]. This development is of course highly desirable. However, in any application of these refined pseudopotentials, problems arise owing to the complications inherent in many of them.

On the other hand we have noticed that, when a certain property is consistently reproduced by a particular form of pseudopotential, another relevant property may be poorly reproduced by the same potential—this is a very common experience in the application of all pseudopotentials whatever the basis of development. However, the degree of such anomalies may be reduced to a great extent, e.g. by employing full non-

* To Professor W H Young on his 60th birthday.

localities in the electron-ion interaction for many systems; this is primarily because the non-local pseudopotentials are proposed generally within the context of the theory of metals [6]. Now, since these types of pseudopotential consist of a number of parameters, it is obvious that a certain degree of uncertainties always exists in the relevant parametric procedure. Owing to these possible uncertainties and some other complexities in the non-local pseudopotential we still believe that the situation, particularly in the s-p bonded metals, can be improved to a greater extent, even working within the *local* pseudopotentials provided that we pay more attention to the electronic structures of these systems.

In this respect we refer to a recent work by Hoshino and Young [7] where a series of properties of Li has been successfully calculated by employing a point-ion pseudopotential. This potential is generated in such a way that the first part of it is calculated within a full self-consistent field potential and the second part contains a repulsive δ potential treated at the origin; the latter part pseudizes the first part through s scattering alone. Now for the s-p bonded systems we need to extend the pseudizing contribution such that both the s and the p scatterings are pseudized properly with the core.

With this picture in mind we write the effective pseudopotential such that the self-consistent field potential contributes to the first part, the relevant exchange and correlation contribution being calculated in the local density functional approximation [8]. The final contributions that arise from the cancellation of the s and p wave scattering with the respective core are expressed in terms of the appropriate functions; these terms essentially take care of the orthogonalization effects. Subsequently to check the validity of this potential we have calculated a number of metallic properties for certain s-p bonded systems. The application of this potential has been found to be fairly successful in calculating these properties on a single footing.

The layout of the paper is as follows: in section 2 we present a brief description of the construction of the effective potential; in section 3 we present the formulation of the quantities that we plan to calculate; in section 4 we present and discuss the results and finally we make some concluding remarks in section 5.

2. The new potential and relevant formulation

Following Hoshino and Young [7] we write the effective local pseudopotential for a metal of atomic number Z as

$$v(r) = v_H(r) + v_{xc}(r) + v_{\text{orth}}(r). \quad (1)$$

The first term is the Hartree potential due to a nucleus and its core electrons; after spin averaging, this term can be written as

$$v_H(r) = -\frac{Z}{r} + 2 \int \sum_{l=0}^p \frac{|\psi_L(r')|^2}{|r_l - r'|} dr'. \quad (2)$$

Here $-Z/r$ is a coulombic potential due to a nuclear charge of Z and the integration represents an electronic Hartree field arising because of the core electrons; this integration in principle can be expressed in closed form for any metallic system. However, we calculate this term using the self-consistent field approximation [9]. The exchange and correlation term $v_{xc}(r)$ representing the exchange-correlation potential between the core and valence electrons is calculated in the local density functional approximation [8]; in the present case we adopt the expression due to Hedin and Lundqvist [10].

The first term $v_{\text{ortho}}(r)$ in equation (2) is the potential generated by orthogonalization of the valence wavefunctions with the core orbitals. Now the appearance of any non-zero amplitude at the origin is due to this core orthogonalization. For a system in which the orthogonalization is affected by the s component of the wavefunctions alone, the relevant orthogonal contribution is represented by a δ function repulsion at the core [7, 11], but for an s-p bonded system this (orthogonalization) is affected by both the s and the p wave scattering and, therefore, the total orthogonalization is now represented by (for details see appendix A)

$$v_{\text{ortho}}(r) = \alpha\delta(r) + \beta\nabla^2\delta(r) \quad (3)$$

where the first term takes care of the s orthogonalization and the second term that arising predominantly from the p waves; any residual orthogonalization due to the s waves is also taken care of by the second term. Here α and β are the parameters signifying the strengths of the s and s-p wave scatterings, respectively, and these are obtained by the usual fitting procedure (for further remarks see section 5).

Now for many practical purposes we need the Fourier transform (FT) of the effective potential. Primarily the FT of the pseudopotential $v(q)$ is used to calculate the effective pairwise potential

$$\varphi(r) = \frac{z^2}{r} + \frac{1}{(2\pi)^3} \int_0^\infty F(q) \frac{\sin(qr)}{qr} 4\pi q^2 dq \quad (4)$$

where z is the valence of the metal concerned. The wavenumber characteristic $F(q)$ is

$$F(q) = (q^2/4\pi)[1/\varepsilon(q) - 1]v^2(q). \quad (5)$$

In the present investigation, $v(q)$ has the form (for details see appendix B)

$$v(q) = v_{\text{ion}}(q) + \alpha - \beta q^2. \quad (6)$$

Here the screening function $\varepsilon(q)$ is calculated in terms of the Lindhard function $\chi_0(q)$ and the Ichimaru-Utsumi [12] local field factor; the latter satisfies the self-consistent conditions imposed by the compressibility sum rule and the short-range correlation requirement.

3. Applications of the point pseudizing potential

In this section we shall describe certain applications of the new pseudopotential whose FT is given by equation (6); the ionic part $v_{\text{ion}}(q)$ is calculated simply by taking the FT of the ionic potential $v_{\text{ion}}(r)$ obtained self-consistently via the modified Herman-Skillman program [13]. When calculating the solid and liquid state properties the density of a hot crystal is assumed to be the same as that of the melting state.

3.1. Cores and related properties

It is now quite well established [14] that a hard-sphere model can describe the liquid state properties of simple metals and their alloys fairly well. In calculating these properties, however, we need the best possible values of the hard-sphere ingredients η and σ . There are various schemes [14] for determining these hard-sphere ingredients. In the present investigation we estimate these values from the consideration that the difference

between the relevant pair potential and its minimum value is just equal to the kinetic energy of a free particle. The standard variational method [15] for defining the hard-sphere ingredients can safely be replaced by the thermodynamic argument proposed by Ashcroft and Langreth [16]. According to their proposal,

$$\varphi(\sigma) - \varphi_{\min}(r) = \frac{3}{2}kT \quad (7)$$

where $\varphi_{\min}(r)$ is the minimum value of $\varphi(r)$. The value of σ thus estimated can be used to calculate the packing fraction η for a particular density n via the relation $\eta = (\pi/6)n\sigma^3$. This optimum value of η is used to calculate the excess entropy per ion [17]:

$$\Delta S_{\text{ex}}/Nk = -\eta(4 - 3\eta)/(1 - \eta)^2. \quad (8)$$

The determination of $\Delta S_{\text{ex}}/Nk$ is an accuracy test for the proposed pseudopotential.

Determination of the Einstein temperature Θ_E is also quite supplementary to that of calculating the excess entropy. Following Hasegawa and Young [18] we write

$$\Theta_E = \frac{\hbar^2}{3k^2M} \sum_{\mathbf{R} \neq 0} (\nabla^2 \varphi)_{\mathbf{R}} = \frac{1.823 \times 10^7}{W} \sum_{\mathbf{R} \neq 0} \left(\frac{d^2 \varphi}{dr^2} + \frac{2}{r} \frac{d\varphi}{dr} \right)_{\mathbf{R}} \quad (9)$$

where \mathbf{R} is a lattice vector of the underlying lattice and W is the atomic weight of the element concerned.

3.2. The tail and the isothermal compressibility

We analyse the accuracy of the tail of the calculated pair potential by estimating the isothermal compressibility χ_r of the systems. In fact we compute the zero-argument structure factor $S(0) = nkT\chi_r$ to check the size of the tail. Following the standard Weeks–Chandler–Andersen (WCA) [19] method it is customary to segregate the pair potential into the core and tail parts [7]. By using this method the WCA diameter of the specimen can be written as [20]

$$\varphi_c(\sigma_{\text{WCA}})/kT = \ln\{-2\sigma_{\text{WCA}}\varphi'_c(\sigma_{\text{WCA}})/kT + Y + 2\}/[-\sigma_{\text{WCA}}\varphi'_c(\sigma_{\text{WCA}})/kT + Y + 2] \quad (10)$$

where $Y = \{\partial\{\ln[g_{\text{hs}}(r)]\}/\partial(\ln r)\}_{\sigma_{\text{WCA}}} + 0$, $g_{\text{hs}}(r)$ being the hard-sphere radial distribution function defined by σ_{WCA} . Using the Percus–Yevick approximation, Y can be written in a closed form [7]. Thus the solution of the transcendental equation (10) gives the WCA diameter σ_{WCA} ; this value is then used to calculate $S_{\text{hs}}(0)$, the zero argument of the hard-sphere structure factor. Finally $S_{\text{hs}}(0)$ expressed within the random-phase approximation is given by

$$S_{\text{RPA}}^{-1}(0) = S_{\text{hs}}^{-1}(0) + S_{\text{t}}^{-1}(0) \quad (11)$$

where

$$S_{\text{t}}^{-1}(0) = (n/kT)\varphi_{\text{t}}(0).$$

Here $\varphi_{\text{t}}(0) = \int_0 \varphi_{\text{t}}(r)4\pi r^2 dr$, $\varphi_{\text{t}}(r)$ being the tail of the pair potential within the WCA approximation. It is relevant to mention here that, owing to the inclusion of softness, σ_{WCA} is naturally greater than the hard-sphere diameter σ .

4. Results and discussion

We have presented the calculated results for Na and Mg in tables 1 and 2 respectively; the results for some other s-p bonded metals are available from the present authors. From table 1 we note that, for Na, most of the desired thermodynamic properties are reproduced consistently by fitting $\alpha = 68.22$ au and $\beta = 27.30$ au in the form factor. The results in table 2 for Mg with $(\alpha, \beta) = (58.65, 13.10)$ show a similar trend. Here we may mention that the process of determining the optimal values of α and β is somewhat tedious. Any small change in these parameters may substantially change the desired physical properties, indicating the sensitivity of the orthogonalization relevant to the form factors.

The consistent reproduction of the hard-sphere ingredients (η, σ) reveals a great degree of accuracy in the profile of the pair potentials calculated by using the present pseudopotential. The hard-sphere ingredients thus determined have been used to calculate the electrical resistivity ρ_1 and excess entropy $\Delta S_{ex}/Nk$; the results for liquid Na and Mg are presented in the tables. These results reveal that the repulsive part and the minimum of the pair potential are consistently reproduced. The random-phase approximation values of the zero-argument structure factor $S_{RPA}(0)$ seem to be fairly consistent with the experimental results and this implies that the tail of the pair potential for the s-p bonded system is also consistently reproduced by the present pseudopotential. From these observations we may remark at this point that the overall profile of the calculated pair potentials is correctly reproduced. From a comparison of the present results with those calculated by using the Ashcroft pseudopotential [21] the greater success of the present potential in calculating the liquid properties is evident.

A similar trend is noticed in the solid state results, e.g. the Einstein temperature Θ_E and band gap v_g for the systems concerned. To avoid any confusion we should mention here that an experimental band gap v_g has a specific value on a particular crystallographic plane and so the comparison may lose its validity to some extent. So far as the Einstein temperature is concerned, it can only be accurately calculated provided that the radial and tangential forces, as represented, respectively, by the first and second derivatives of φ (see equation (9)) are correctly reproduced. The calculated results show fair consistency in comparison with the values obtained by using the other established pseudopotentials.

Let us now analyse the appealing features generated by the present potential in comparison with those generated by other established potentials, e.g. the Ashcroft potential. In any empty-core or nearly-empty-core potential the point-ion part is usually a purely coulombic potential, indicating that the valence electrons see a fully screened core at all separations. This approximation, even though it works quite well for certain ideal cases, fails to reproduce the reality of the physical aspects exhibited in any electron screening. Ideally the valence electrons in the close vicinity of the respective nucleus see all the protons without any appreciable screening and on the other hand electrons from large separations experience only the positive core having charges just equal but opposite to the valence electrons. These practical features are fully generated by the present point-ion part comprising the self-consistent Hartree and the exchange-correlation contributions in the total potential.

In figures 1(a) and 2(a) are shown the pseudopotential form factors for Na and Mg calculated by using the present point-ion pseudizing potential. Since the asymptotic behaviours of all the hitherto-known pseudopotentials are similar, we obviously notice an identical feature in the long-wavelength region of all the corresponding form factors.

Table 1. Calculated values of the various properties relevant to the solid and liquid phases of Na for certain values of the strength parameters α and β . For comparison the results obtained by using the Ashcroft empty-core pseudopotential with different values of r_c are also presented in the bottom half of the table. Details of the physical quantities are presented in the text. Relevant experimental values are given within parentheses. Unless otherwise stated, all dimensional quantities are expressed in atomic units. Calculations use the melting point ($T = 371$ K) value of the number density $n = 3.583 \times 10^{-2}$ au.

α	β	σ	η	σ_{wca}	η_{wca}	$S_{hd}(0)$	$S_n(0)$	$S_{RPA}(0)$	δ_l ($\mu\Omega$ m)	$-\Delta S_{ex}/Nk$	v_t (Ryd)	Θ_E (K)
68.22	27.30	6.246	0.459 (0.46) ^a	6.473	0.5105	0.014 05	-0.024 14	0.033 61 (0.023) ^b	9.45 (9.57) ^c	4.114 (3.490) ^d	0.0073 (0.0079) ^e	80 (106) ^b
68.50	27.30	6.277	0.466	6.475	0.5111	0.014 09	-0.025 50	0.031 49	10.374	4.252	0.0062	79
67.50	27.00	6.171	0.442	6.362	0.4850	0.018 13	-0.025 94	0.060 22	9.185	3.796	0.006	77
$r_c = 1.60$		5.706	0.350	5.940	0.395	0.042 00	-0.159 46	0.057 02	18.491	2.444	-0.0002	92
1.67		5.892	0.385	6.126	0.433	0.029 76	-0.148 92	0.037 18	13.926	2.896	-0.0002	84
1.85		6.372	0.487	6.583	0.537	0.010 68	-0.119 91	0.011 72	9.614	4.698	-0.0001	127

^a From Waseda [22].

^b From Young [23].

^c From Shimoji [24].

^d From Hultgren *et al.* [25].

^e From Cohen and Heine [26].

^f The empty-core radius $r_c = 1.67$ au corresponds to the liquid state resistivity data [26] and other values for r_c are chosen quite randomly [27].

Table 2. Calculated values of the various properties relevant to the solid and liquid phases of Mg for certain values of the strength parameters α and β . For comparison the results obtained by using the Ashcroft empty-core pseudopotential with different values of τ_c are also presented in the bottom half of the table. Details of the physical quantities are presented in the text. Relevant experimental values are given within the parentheses. Unless otherwise stated all dimensional quantities are expressed in atomic units. Calculations use the melting point ($T = 923$ K) value of the number density $n = 5.836 \times 10^{-3}$ au.

α	β	σ	η	σ_{WCA}	η_{WCA}	$S_{in}(0)$	$S_s(0)$	$S_{RPA}(0)$	δ_1 ($\mu\Omega$ m)	$-\Delta S_{in}/Nk$	v_g (Ryd)	Θ_E (K)
58.65	13.10	5.330	0.463 (0.46) ^a	5.463	0.498	0.015 90	-0.044 210	0.029 71 (0.025) ^b	26.15 (27.40) ^c	4.192 (3.410) ^d	0.012 (0.007) ^e	177 (170) ^b
58.00	12.70	5.289	0.452	5.417	0.486	0.018 00	-0.033 89	0.038 40	28.32	3.980	0.008	126
56.00	16.30	5.323	0.461	5.467	0.499	0.015 71	-0.056 84	0.021 71	27.20	4.153	0.010	117
$\tau_c = 1.39$		5.318	0.460	5.646	0.550	0.009 32	-0.384 47	0.009 55	19.29	4.133	0.009	243
1.44		5.424	0.488	5.744	0.579	0.006 7	-0.2312	0.006 90	27.15	4.721	0.011	(281)

^a From Waseda [22].

^b From Young [23].

^c From Shimoji [24].

^d From Hultgen *et al* [25].

^e From Cohen and Heine [26].

^f The empty-core radius $\tau_c = 1.39$ au corresponds to the liquid state resistivity data [26] and the other value for τ_c is chosen quite randomly [27].

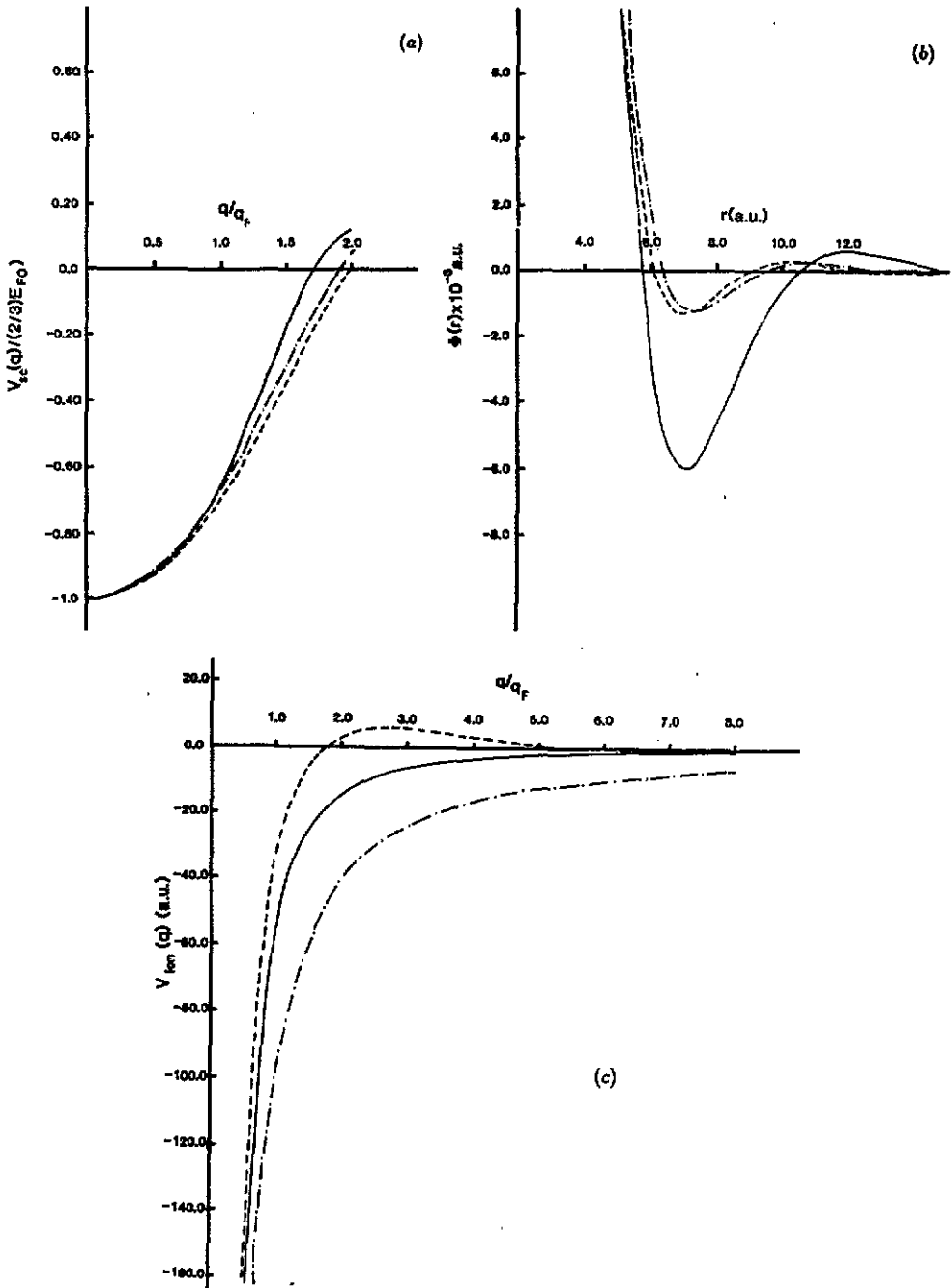


Figure 1. (a) Screened and normalized pseudopotential form factors for Na: —, present form factor with the strength parameters $\alpha = 68.22$ au and $\beta = 27.30$ au; ---, Ashcroft potential with empty-core radius $r_c = 1.67$ au; — · —, Ashcroft potential with $r_c = 1.75$ au. (b) The pair potentials $\phi(r)$ calculated using the form factors shown in (a): the curves have the same meanings as those in (a). (c) Unscreened ionic form factors: — · —, present results; ---, Ashcroft form factor with $r_c = 1.75$ au; —, purely coulombic form factor. All these results correspond to the melting point ($T = 371$ K) number density $n = 3.583 \times 10^{-3}$ au for Na.

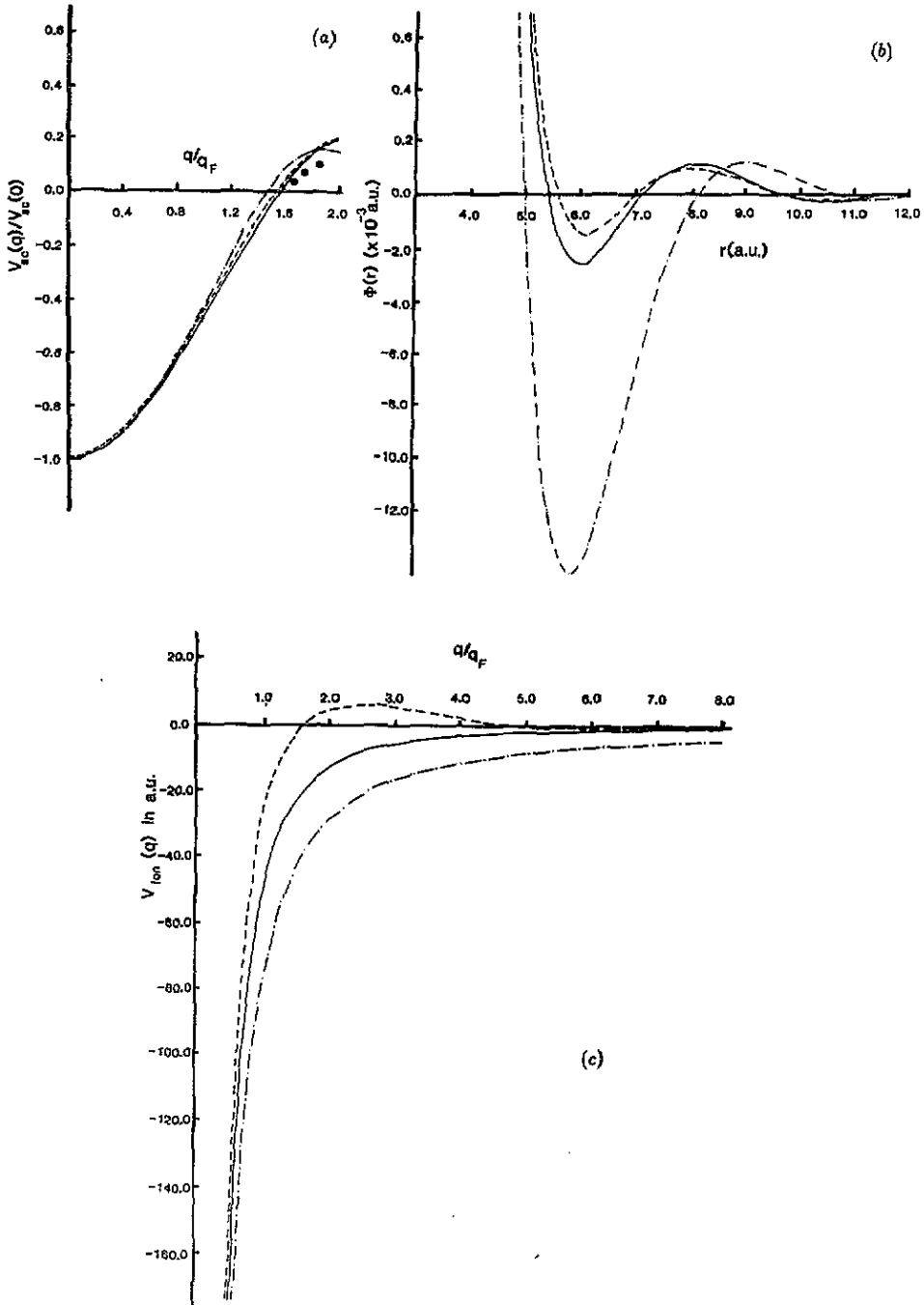


Figure 2. (a) Screened and normalized pseudopotential form factors for Mg: —·—, present form factor with strength parameters $\alpha = 58.65$ au and $\beta = 13.10$ au; —, Ashcroft potential with empty-core radius $r_c = 1.39$ au; - - -, Ashcroft potential with $r_c = 1.44$ au. (b) The pair potentials $\phi(r)$ calculated using the form factors shown in figure (a): The curves have the same meanings as in (a). (c) Unscreened ionic form factors: —·—, present results; - - -, Ashcroft form factor with $r_c = 1.39$ au; —, purely coulombic form factor. All these results correspond to the melting point ($T = 923$ K) number density $n = 5.836 \times 10^{-3}$ au for Mg.

However, differences in the large q region appear because of the way in which the valence electrons view the ion core; this is certainly obvious. In this respect we may mention that one of the striking aspects of the pair potentials, as shown in figures 1(b) and 2(b), is the significantly deep minimum associated with each of them. This feature may be a consequence of the differences between the profiles of the present and other ionic potentials appearing in the metallic range of separation r . This is reflected in the ionic bare form factors, as shown in figures 1(c) and 2(c), calculated using the various pseudopotentials. At this stage it is not, however, clear how much these deep minima are due to the differences between the asymptotic behaviour of the ionic potentials and the relevant orthogonalization contributions.

5. Conclusions

In the present attempt we have developed a local pseudopotential suitable for the s-p bonded systems. With a proper choice of the two strength parameters α and β we have been able to calculate successfully a number of properties relevant to the solid and liquid phases of a few of these systems. In the light of the calculated results we would like to make the following concluding remarks.

(i) In the first place, the present pseudopotential is local but consists of the full electron-ion interaction; the latter is absent in most of the hitherto-known local pseudopotentials for the s-p bonded systems. The essential feature of this description is the occurrence of the true field rather than a coulombic form.

(ii) The full self-consistency inherent in the ionic part of the pseudopotential ensures exact description of the electron screening. This feature on the contrary represents an ideal band description essential for any electron-ion interaction.

(iii) The equally good core and tail of the pair potential imply that the interatomic interactions are correctly represented by the present pseudopotential. These features indicate that the deep minima associated with the pair potentials do not have any unwanted effect on the thermodynamic properties of the systems concerned. However, any other relevant property probing critically the effects due to the details of the potential well remains to be investigated.

(iv) Despite all its appealing features, the pseudopotential form factor calculated by using the present point-ion pseudizing potential has two difficult features: one arising from the constant term α , for in this case $v(q)$ does not tend to zero as $q \rightarrow \infty$ and the other is related to the q^2 -dependent term in $v(q)$. These features, however, will not affect any property involving the electron scattering by the Fermi surface. Nonetheless, global properties, e.g. the free energy, may be wrongly reproduced by the present pseudopotential unless the said features are neutralized by some relevant factors. Some appropriate corrections may be made to these difficulties following the recent work by Das and Joarder [28].

(v) At this stage we should mention that the strength parameters α and β , even though at present treated as disposable quantities, may be calculated in terms of any first-principles method; the latter may be achieved by considering bound-state properties of the elemental systems. At that stage it will be appropriate to check for further validity of the proposed values of α and β , e.g. by fitting these to atomic properties to, say, atomic levels of the relevant atoms or ions.

Work considering the above points is in progress.

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Appendix A. Pseudizing potential based on the δ function

In terms of the so-called jellium model [1] a metal is described as a collection of electrons distributed uniformly in a compensating positive-charge background. Now, if the background is replaced by a collection of discrete ions, the distributed electrons will find themselves in a different average field. This differing situation introduces a perturbation in the electron-ion interaction. If this perturbation is weak, we may represent it by a pseudopotential v_{ps} . Thus in terms of the given ionic potential v_{ion} the form factor of the effective potential is written as

$$\langle k | v_{ps} + v_{ion} | k + q \rangle = \langle k | v_{ps} | k + q \rangle + \langle k | v_{ion} | k + q \rangle = v_{ps}(q) + v_{ion}(q). \quad (A1)$$

In general we may write

$$\langle k | v_{ps} | k + q \rangle = \frac{1}{k} \sum_{l=0}^{\infty} (2l + 1) \eta_l p_l(\cos \theta) \quad (A2)$$

where the notation has its usual meanings. We may write

$$\langle k | v_{ps} | k + q \rangle = \int v_{ps}(r) \exp(iq \cdot r) dr. \quad (A3)$$

If we consider v_{ps} to cancel s scattering alone, then

$$v_{ps}^s(r) = \alpha \delta(r) \quad (A4)$$

because then

$$\int v_{ps}^s(r) \exp(iq \cdot r) dr = \alpha. \quad (A5)$$

Here α is a strength parameter and in principle it depends on energy via k , but we have not explicitly shown this here.

On the other hand, if $v_{ps}(r)$ is to cancel the p wave and any residual s wave scattering, then

$$v_{ps}^p(r) = \beta \nabla^2 \delta(r). \quad (A6)$$

Thus for effective s-p scattering we may write

$$v_{ps}(r) = (\alpha + \beta \nabla^2) \delta(r) \quad (A7)$$

which is essentially the total orthogonalization contribution v_{ortho} given by equation (3) in the main text.

Appendix B. Form factor of the effective pseudopotential

The effective pseudopotential is

$$v(\mathbf{r}) = v_{\text{ion}}(\mathbf{r}) + v_{\text{ps}}(\mathbf{r}) \quad (\text{B1})$$

where

$$v_{\text{ion}}(\mathbf{r}) = v_{\text{H}}(\mathbf{r}) + v_{\text{xc}}(\mathbf{r}) \quad (\text{B2})$$

as defined in equation (1). Combining equations (A7) and (B2), and finally taking their FT, we have

$$v(\mathbf{q}) = v_{\text{ion}}(\mathbf{q}) + v_{\text{ps}}(\mathbf{q}). \quad (\text{B3})$$

Here

$$v_{\text{ps}}(\mathbf{q}) = \int \alpha \delta(\mathbf{r}) \exp(i\mathbf{q} \cdot \mathbf{r}) \, d\mathbf{r} + \int \beta \nabla^2 \delta(\mathbf{r}) \exp(i\mathbf{q} \cdot \mathbf{r}) \, d\mathbf{r} \quad (\text{B4})$$

where, as already defined,

$$\int \alpha \delta(\mathbf{r}) \exp(i\mathbf{q} \cdot \mathbf{r}) \, d\mathbf{r} = \alpha.$$

In the present case we assume $\beta \nabla^2 \delta(\mathbf{r})$ to be spherically symmetric and so

$$\int \beta \nabla^2 \delta(\mathbf{r}) \exp(i\mathbf{q} \cdot \mathbf{r}) \, d\mathbf{r} = \beta \int \left(\frac{1}{r} \frac{d^2}{dr^2} \delta(r) \right) \frac{\sin(qr)}{(qr)} 4\pi r^2 \, dr = -\beta q^2. \quad (\text{B5})$$

Thus the FT of $v(\mathbf{r})$ is given by

$$v(\mathbf{q}) = v_{\text{ion}}(\mathbf{q}) + \alpha - \beta q^2 \quad (\text{B6})$$

which is essentially equation (6) in the text.

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