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2008 J. Phys.: Condens. Matter 20 114111

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The Wills–Harrison approach to the thermodynamics of binary liquid transition-metal alloys

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Received 30 August 2007, in final form 9 October 2007

Published 20 February 2008

Online at stacks.iop.org/JPhysCM/20/114111

Abstract

In the present study, the Wills–Harrison approach in conjunction with the Bretonnet–Silbert local model pseudopotential is applied to the thermodynamics of binary transition-metal liquid alloys. The calculation is performed in the framework of the variational method of thermodynamic perturbation theory with a hard-sphere reference system. The Vashishta–Singwi exchange–correlation function and the Nozières–Pines exchange–correlation energy are used. The free energy of mixing for liquid Fe–Co alloy is calculated at different compositions near the melting temperature. The agreement with the experimental data is quite satisfactory.

1. Introduction

The strict theory of simple liquid metals is rather well developed. Existing methods allow one to investigate successfully the simple metal liquid binary alloys also, including thermodynamics (Umar *et al* 1974, Singh 1980, Hafner 1987, Dubinin *et al* 1998 etc). For liquid alloys of transition metals, the situation is much poorer. The investigations of liquid transition metals in the frameworks of electron theory and the theory of liquids started from the works of Yuryev (1985) and Aryasetiawan *et al* (1986). In both of these works, the variational method of thermodynamic perturbation theory (TPT) with a hard-sphere (HS) reference system was used. Yuryev (1985) used the non-local model pseudopotential (MP) to describe the electron structure, while in the paper of Aryasetiawan *et al* (1986), the tight-binding model of Ducastelle (1970) was applied.

Further development of the theory deals with the Wills–Harrison (WH) approximation (Wills and Harrison 1983). This approximation suggests separate description of the s- and d-electron states. The first is described as a nearly free-electron (NFE) state, while the second one is suggested to be completely localized, so that the atomic position is supposed to be a good quantum number for the d-electron state. The WH approach to the liquid transition metals was first applied by Hausleitner and Hafner (1988). In the above work, the pair correlation function $g(r)$, the structure

factor $S(q)$, the free energy F , and the entropy S for the 3d transition metals were calculated with the HS and HS Yukawa reference systems. Regnaut (1989) combined the WH approach with the Weeks–Chandler–Andersen (Weeks *et al* 1971) method and with the optimized random phase approximation (ORPA) to calculate structural characteristics of certain liquid transition metals. Later, Bretonnet and Derouiche (1991) calculated the free energy of 3d, 4d and 5d liquid transition metals by the HS variational method. The analysis of the validity of the WH approach to the liquid state was summarized by Hausleitner *et al* (1991), where the $g(r)$ and $S(q)$ obtained using different TPT approximations, different integral equations, and molecular dynamics (MD) simulations were compared. Earlier (Hausleitner and Hafner 1988), it was shown that in the frameworks of variational methods the best coincidence with experiment is achieved for the middle-row transition metals (with half-filled d shell). In contrast, Hausleitner *et al* (1991) stated an inverted tendency for the ORPA and some integral equations. As regards MD, the best agreement with experiment was achieved for Fe, Co, and Ni. The same was stated for Zerah and Hansen (1986) thermodynamically self-consistent approximation. Thus, it may be concluded that the WH potential may, in principle, be applied for a quantitative description of liquid transition metals, especially of the iron group.

Bretonnet and Silbert (1992) (BS) have used the Oli local MP (Oli 1988), which was designed especially for transition

metals. They modified the Oli potential, so below it will be referred to as the BS model potential. The BS MP has been applied to calculate structural and thermodynamic characteristics of liquid transition metals (Bretonnet *et al* 1992, Bhuiyan *et al* 1992, Jakse and Bretonnet 1995, Jakse *et al* 1996). Since, in the WH formalism, the simplest empty-core (Ashcroft 1966) MP is usually used, it seems that the BS MP may be considered as a better approximation for the NFE part of the calculation.

Thus, in the present work, we use the BS MP instead of the Ashcroft one in the WH formalism. A combined WH–BS approach for the HS variational method is derived. The formalism does not deal with the approximate shape of the WH pair potential and implies all energetic contribution calculations in the wave space. Also, we derive the generalization of the formalism to the binary alloys and calculate the thermodynamic characteristics of liquid Fe–Co system.

2. The WH approximation; generalization to binary systems

The basis of the WH approximation is the suggestion that the wavefunctions of the hybridized s–d band may be approximated as a superposition of the plane waves and the d functions of a free atom. This means that conductive electrons may be divided into s and d ones.

The s electrons behave as if nearly free and may be described in the NFE approximation with some perturbing pseudopotential as in the simple metal theory. The difference is that one has to use the effective valence z_s instead of the number of valence s electrons per ion. Due to the s–d hybridization z_s is less than the number of valence s electrons in a free atom.

The d electrons are practically localized near the atom. In the second order of perturbations, the shift of the d-electron energy of the metal with respect to the single atom is (Harrison and Froyen 1980)

$$V_{dd'} = \sum_{\vec{k}} \frac{\langle d|\Delta|\vec{k}\rangle\langle\vec{k}|\Delta|d'\rangle}{e_d - e_{\vec{k}}}, \quad (1)$$

where d and d' states are localized on different atoms, Δ is the difference between d-electron potentials in the metal and in the single atom (it may be treated as a perturbation which causes the transition from the d state into the s state), $|\vec{k}\rangle$ is the plane-wave function, e_d is the energy of the unperturbed d state, $e_{\vec{k}}$ is the plane-wave energy.

If one takes the muffin-tin (MT) potential (Andersen 1975) in the atomic sphere approximation (Mackintosh and Andersen 1979) as a metal ion–electron potential, then from (1) one gets mean potential of the d–d interaction, $V_d(r)$ (hereafter in atomic units):

$$V_d(r) = \frac{28.06r_d^3}{\pi r^5}, \quad (2)$$

where r_d is the d-state radius, which is the characteristic of a free atom.

Since the Δ in (1) is small enough, the d-electron contribution to the density of states corresponds to a narrow peak. The width of the peak W_d may be calculated as a second moment of the d-state density $n_d(\varepsilon)$. Using (1), one gets

$$W_d = \left(\frac{12}{N} \sum_{m=1}^N \sum_{\substack{l=1 \\ l \neq m}}^N V_d^2(\vec{r}_{ml}) \right)^{1/2}, \quad (3)$$

where N is the number of atoms.

For the peak of $n_d(\varepsilon)$, Wills and Harrison (1983) used rectangular approximation (Friedel 1969):

$$n_d(\varepsilon) = \begin{cases} 10/W_d, & \varepsilon_d - W_d/2 \leq \varepsilon \leq \varepsilon_d + W_d/2 \\ 0, & \text{other } \varepsilon, \end{cases} \quad (4)$$

where ε_d is the center of gravity of the d band.

The d-electron contribution to the internal energy per atom E_d may be calculated in a standard way:

$$E_d = \int_{\varepsilon_d - W_d/2}^{\varepsilon_F} n_d(\varepsilon) f(\varepsilon) \varepsilon d\varepsilon \\ = E_b + E_c = -\frac{1}{2} z_d \left(\frac{10 - z_d}{10} \right) W_d + z_d \varepsilon_d, \quad (5)$$

where ε_F is the Fermi energy, z_d is the effective number of valence d electrons per atom ($z_d = z - z_s$, where z is the total number of valence electrons per atom), $f(\varepsilon)$ is the Fermi distribution function.

For the E_c , which corresponds to the ε_d shift with respect to the energy of the single-atom d state, the following first-order approximation is used in the WH approach:

$$|D\rangle = |d\rangle + \sum_{\vec{k}} |\text{OPW}_{\vec{k}}\rangle \frac{\langle\vec{k}|\Delta|d\rangle}{e_d - e_{\vec{k}}}, \quad (6)$$

where $|\text{OPW}_{\vec{k}}\rangle$ is the orthogonalized plane wave.

The overlap between perturbed d states is

$$S_{dd'} = \delta_{dd'} + \sum_{\vec{k}} \frac{\langle d|\Delta|\vec{k}\rangle\langle\vec{k}|\Delta|d'\rangle}{(-k^2/2)^2}. \quad (7)$$

Then, one gets, like (3) and (2),

$$\varepsilon_d = \frac{1}{2N} \sum_{m=1}^N \sum_{\substack{l=1 \\ l \neq m}}^N V_S(\vec{r}_{ml}), \quad (8)$$

$$V_S(r) = \frac{225r_d^6}{\pi^2 r^8}. \quad (9)$$

As may be derived from (5), (8), (9),

$$E_c = z_d 2\pi\rho \int_0^\infty \frac{225r_d^6}{\pi^2 r^8} g(r) r^2 dr, \quad (10)$$

where ρ is the number atomic density.

From (10) one can derive the corresponding contribution to the effective pair potential:

$$\varphi_c(r) = z_d \frac{225r_d^6}{\pi^2 r^8}. \quad (11)$$

For E_b (see (3)), this cannot be done in an explicit form:

$$E_b = -\frac{1}{2}z_d \left(\frac{10 - z_d}{10} \right) \sqrt{12} \left(4\pi\rho \int_0^\infty V_d^2(r)g(r)r^2 dr \right)^{1/2}. \quad (12)$$

Thus, only two parameters are necessary for the calculation of the d-electron contribution to the internal energy: the d-state radius r_d and the effective number of d electrons per atom z_d . Let us mention that r_d may be treated as a phenomenological parameter. Wills and Harrison (1983) have determined it from the solution of the Schrödinger equation with the MT potential of a single atom. For the metal, however, d states correspond to the conductive band, so one can expect some rise of r_d .

Below, the generalization of above formulas to the binary alloy is given (in atomic units per atom) by

$$E_b = -\frac{1}{2}\bar{z}_d \left(\frac{10 - \bar{z}_d}{10} \right) W_d, \quad (13)$$

$$W_d = \sqrt{12} \left(4\pi\rho \sum_{i,j=1}^2 c_i c_j \int_0^\infty V_{dij}^2(r)g_{ij}(r)r^2 dr \right)^{1/2}, \quad (14)$$

$$V_{dij}(r) = \frac{28.06(r_{di}r_{dj})^{3/2}}{\pi r^5}, \quad (15)$$

$$E_c = 2\pi\rho \sum_{i,j=1}^2 c_i c_j \int_0^\infty \varphi_{cij}(r)g_{ij}(r)r^2 dr, \quad (16)$$

$$\varphi_{cij}(r) = \bar{z}_d \frac{225(r_{di}r_{dj})^3}{\pi^2 r^8}, \quad (17)$$

where $g_{ij}(r)$ are the partial pair correlation functions, r_{di} is the radius of the d state for the atom of the i th kind, c_i is the concentration of the i th component, z_{di} is the effective number of valence d electrons per i th kind of atom, $\bar{z}_d = c_1 z_{d1} + c_2 z_{d2}$.

3. The Bretonnet–Silbert model potential

Oli's idea arises from the work of Swan (1967), where the inverse scattering task of reconstructing the potential from the phase shifts has been performed. It was shown that it is possible to restrict the potential to the first two terms of the Dirichlet series.

The local Oli MP accounts for the s–d scattering inside the ion core r_c , while outside r_c , the Coulomb ion–electron potential is suggested (in atomic units) as

$$\omega_O(r) = \begin{cases} \sum_{n=1}^2 B_n \exp\left(-\frac{r}{nr_c}\right), & r \leq r_c \\ -z_s/r, & r > r_c, \end{cases} \quad (18)$$

where B_1 and B_2 are the Dirichlet coefficients.

For the BS MP, some arbitrary a has been used instead of r_c in the series exponents in (18). The coefficients B_1, B_2 have to be chosen so as to make the potential and its first derivative

continuous at $r = r_c$:

$$\omega_{BS}(r) = \begin{cases} \sum_{n=1}^2 B_n \exp\left(-\frac{r}{na}\right), & r \leq r_c \\ -z_s/r, & r \geq r_c, \end{cases} \quad (19)$$

$$B_1 = (z_s/r_c)[1 - 2a/r_c] \exp(r_c/a),$$

$$B_2 = (2z_s/r_c)[a/r_c - 1] \exp(0.5r_c/a).$$

The BS MP unscreened ion form factor is

$$\omega_{BS}(q) = 4\pi\rho a^3 \left[\frac{B_1 J_1(q)}{(1 + a^2 q^2)^2} + \frac{8B_2 J_2(q)}{(1 + 4a^2 q^2)^2} \right] - (4\pi z_s \rho / q^2) \cos(qr_c),$$

$$J_1(q) = 2 - \exp\left(-\frac{r_c}{a}\right) \left\{ \left[r_c \frac{1 + a^2 q^2}{a} + 1 - a^2 q^2 \right] \frac{\sin(qr_c)}{aq} + \left[2 + \frac{r_c(1 + a^2 q^2)}{a} \right] \cos(qr_c) \right\}, \quad (20)$$

$$J_2(q) = 2 - \exp\left(-\frac{r_c}{2a}\right) \left\{ \left[r_c \frac{1 + 4a^2 q^2}{2a} + 1 - 4a^2 q^2 \right] \frac{\sin(qr_c)}{2aq} + \left[2 + \frac{r_c(1 + 4a^2 q^2)}{2a} \right] \cos(qr_c) \right\}.$$

For the binary system, expressions (19), (20) may be rewritten in a straightforward way by using characteristics of the i th kind of ion ($i = 1, 2$): z_{si}, r_{ci} and a_i (Dubinin *et al* 2007).

4. The WH approach for binary systems in the framework of the HS variational method

To examine the applicability of above described approach to the quantitative description of binary liquid transition-metal alloy thermodynamics, we use the simplest (but well proved for simple metals) thermodynamic perturbation theory variational method, with a hard-sphere reference system (Mansoori and Canfield 1969). The method is based on the following inequality (in atomic units per atom):

$$F \leq F_{HS} + U_e + \langle U_1 \rangle_{HS} - T S_e, \quad (21)$$

where U_e is the s-electron energy contribution which does not depend on the structure, U_1 is the potential energy perturbation, S_e is the electron entropy, $F_{HS} = 3k_B T/2 - T S_{HS}$, S_{HS} is the entropy of the HS system (for a binary system it has been obtained in an analytical form by Umar *et al* 1974).

For a transition-metal binary alloy, the potential energy perturbation averaged over the HS reference system may be written as

$$\langle U_1 \rangle_{HS} = 2\pi\rho \sum_{i,j=1}^2 c_i c_j \int_{\sigma_{ij}}^\infty g_{ijHS}(r)\varphi_{ijNFE}(r)r^2 dr + \langle E_d \rangle_{HS}, \quad (22)$$

where the σ_{ij} are the partial HS diameters, $\varphi_{NFE}(r)$ is the s-electron contribution to the effective pair interaction:

$$\varphi_{ijNFE}(r) = \frac{z_{si}z_{sj}}{r} + \frac{1}{8\pi^2\rho} \int_0^\infty F_{ij}(q) \frac{\sin(qr)}{qr} q^2 dq, \quad (23)$$

where z_{si} is the effective number of valence s electrons per i th kind of ion (taken here as for pure metals), $F_{ij}(q)$ are the partial energy–wavenumber characteristics:

$$F_{ij}(q) = -\frac{q^2}{\pi\rho}\omega_i(q)\omega_j(q)[(\varepsilon_H(q) - 1)^{-1} + (1 - f(q))]^{-1}, \quad (24)$$

where $\omega_i(q)$ is the pseudopotential form factor of the i th kind of unscreened ion (for which we use the BS MP form), $\varepsilon_H(q)$ is the Hartree dielectric function, $f(q)$ is the exchange–correlation function (for the latter, we use the $f(q)$ suggested by Vashishta and Singwi 1972).

In wave space, the right part of (21) F_{var} has been written as

$$F_{\text{var}} = F_{\text{HS}} + E_0 + E_1 + E_2 + E_M + E_b + E_c - T S_e, \quad (25)$$

where E_0 is the free-electron gas energy, E_1 is the first-order perturbation with respect to pseudopotential, E_2 is the second-order pseudopotential term or the NFE band structure energy, E_M is the Madelung energy:

$$E_0 = 0.3\bar{z}_s k_F^2 - 0.5\bar{z}_s(\pi k_B T/k_F)^2 + E_{\text{NP}}, \quad (26)$$

$$E_1 = \bar{z}_s \sum_{i=1}^2 c_i \lim_{q \rightarrow 0} (\omega_i(q) + 4\pi\rho z_{si}/q^2), \quad (27)$$

$$E_2 = (1/2\pi^2\rho) \sum_{i,j=1}^2 \sqrt{c_i c_j} \int_0^\infty S_{ij\text{HS}}(q) F_{ij}(q) q^2 dq, \quad (28)$$

$$E_M = (1/\pi) \sum_{i,j=1}^2 z_{si} z_{sj} \sqrt{c_i c_j} \int_0^\infty (S_{ij\text{HS}}(q) - \delta_{ij}) dq, \quad (29)$$

where $k_F = (3\bar{z}_s \rho \pi^2)^{1/3}$ is the Fermi wavevector, E_{NP} is the Pines and Nozieres (1966) exchange–correlation energy, $\bar{z}_s = c_1 z_{s1} + c_2 z_{s2}$, $S_{ij\text{HS}}(q)$ are the HS partial structure factors in the Ashcroft and Langreth (1967) (AL) analytical form. For the E_M and E_1 , analytical expressions obtained in the AL approximation by Umar *et al* (1974) and in the BS MP approximation by Dubinin *et al* (2007), respectively, are used.

The E_b and E_c contributions after averaging over the HS system take the form

$$E_b = -\frac{1}{2}\bar{z}_d \left(\frac{10 - \bar{z}_d}{10} \right) \langle W_d \rangle_{\text{HS}}, \quad (30)$$

$$\langle W_d \rangle_{\text{HS}} = \sqrt{12} \left(4\pi\rho \sum_{i,j=1}^2 c_i c_j \int_{\sigma_{ij}}^\infty V_{dij}^2(r) g_{ij\text{HS}}(r) r^2 dr \right)^{1/2}, \quad (31)$$

$$E_c = 2\pi\rho \sum_{i,j=1}^2 c_i c_j \int_{\sigma_{ij}}^\infty \varphi_{cij}(r) g_{ij\text{HS}}(r) r^2 dr. \quad (32)$$

To make the calculations in the wave space, one has, as for the first term in the right side of (22), to use the well-known relation

$$g_{ij}(r) = 1 + \frac{1}{2\pi^2\rho\sqrt{c_i c_j}} \int_0^\infty [S_{ij}(q) - \delta_{ij}] \frac{\sin(qr)}{qr} q^2 dq. \quad (33)$$

Table 1. Input data for the calculation.

	r_{ci} (au)	a_i (au)	z_{si}	z_{di}	Ω (au)	r_{di} (au)
Fe	1.540	0.363	1.4	6.6	89.29	2.3
Co	1.641	0.393	1.4	7.6	85.85	1.9

Table 2. Calculated free energy F (eV) of 0.5 Fe–0.5 Co liquid alloy and contributions to it.

F	$\frac{3}{2}k_B T$	E_0	E_1	E_2	E_M	E_d	$-TS$
–22.810	0.241	–1.736	6.132	–3.517	–17.289	–5.699	–0.942

So that

$$\langle W_d \rangle_{\text{HS}} = \frac{97.2}{\pi} \left(4\pi\rho \sum_{i,j=1}^2 \frac{c_i c_j (r_{di} r_{dj})^3}{7\sigma_{ij}^7} + \frac{2}{\pi} \sum_{i,j=1}^2 \sqrt{c_i c_j} r_{di}^3 r_{dj}^3 \right. \\ \left. \times \int_0^\infty [S_{ij\text{HS}}(q) - \delta_{ij}] q dq \int_{\sigma_{ij}}^\infty \frac{\sin(qr)}{r^9} dr \right)^{1/2}, \quad (34)$$

$$E_c = \bar{z}_d \frac{225}{\pi^2} \left(2\pi\rho \sum_{i,j=1}^2 \frac{c_i c_j (r_{di} r_{dj})^3}{5\sigma_{ij}^5} + \frac{1}{\pi} \sum_{i,j=1}^2 \sqrt{c_i c_j} r_{di}^3 r_{dj}^3 \right. \\ \left. \times \int_0^\infty [S_{ij\text{HS}}(q) - \delta_{ij}] q dq \int_{\sigma_{ij}}^\infty \frac{\sin(qr)}{r^7} dr \right). \quad (35)$$

The integrals in (34), (35) have to be calculated numerically.

The electron entropy has been calculated as

$$S_e = (\pi k_B)^2 T n(\varepsilon_F)/3, \quad (36)$$

where $\varepsilon_F = k_F^2/2$, $n(\varepsilon)$ is the full electron density of states:

$$n(\varepsilon) = n_d(\varepsilon) + \sqrt{\varepsilon}/(2\pi^2\rho). \quad (37)$$

The density of d states may be taken in the rectangular approximation (4), but we use the Lorenz shape which is more suitable here:

$$n_d(\varepsilon) = \frac{10W_d}{\pi[(\varepsilon - \varepsilon_F + W_d/\tan(\pi\bar{z}_d/10))^2 + W_d^2]}. \quad (38)$$

The free energy minimization is over three parameters: the number atomic density ρ and the HS diameters σ_{11} and σ_{22} .

5. Results: application to the Fe–Co system

To estimate the validity of method developed, the thermodynamic properties of the Fe–Co system were calculated at $T = 1863$ K.

The BS MP parameters were those from the work of Jakse and Bretonnet (1995). Parameter r_{di} for each of the pure metals was chosen so as to make the calculated atomic volume Ω coincide with the experimental one (Waseda 1981). All the input data are presented in table 1.

In table 2, all contributions to the calculated free energy per atom at the equiatomic composition are listed.

The results of the mixing free energy calculation in comparison with the experimental data (Hultgren *et al* 1973) are presented at figure 1.

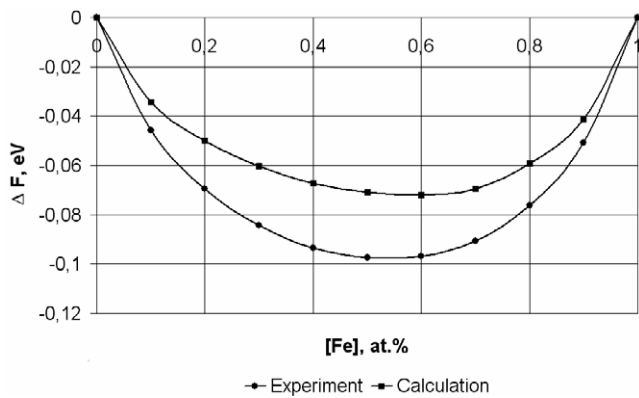


Figure 1. Free energy of mixing per atom for the Fe–Co system.

In spite of there being some mismatch, the results are rather gratifying, since the possibility in principle of the application of the method offered for the quantitative description of binary systems does not leave any doubt. It should be stressed that the qualitative agreement of a fine mixing free energy has been achieved while several possibilities for enhancing the calculations remained unrealized. These are:

- (1) Relating the BS MP parameters and the WH characteristics of d states. The Oli (1988) reverse scattering construction allows one to do this.
- (2) Applying more reliable methods of thermodynamic perturbation theory instead of the HS variational one. The fact is that the effective WH pair potential differs from the HS one more strongly than those in the simple metal theory.

Acknowledgments

We are grateful to RFBR for financial support (grants 05-03-32866 and 07-02-96045r).

References

Andersen O K 1975 *Phys. Rev. B* **12** 3060

- Aryasetiawan F, Silbert M and Stott M J 1986 *J. Phys. F: Met. Phys.* **16** 1419
- Ashcroft N W 1966 *Phys. Lett.* **23** 48
- Ashcroft N W and Langreth D C 1967 *Phys. Rev.* **156** 685
- Bhuiyan G M, Bretonnet J L, Gonzales L E and Silbert M 1992 *J. Phys.: Condens. Matter* **4** 7651
- Bretonnet J L, Bhuiyan G M and Silbert M 1992 *J. Phys.: Condens. Matter* **4** 5359
- Bretonnet J L and Derouiche A 1991 *Phys. Rev. B* **43** 8924
- Bretonnet J L and Silbert M 1992 *Phys. Chem. Liq.* **24** 169
- Dubinin N E, Son L D and Vatolin N A 2007 *Defect Diffus. Forum* **263** 105
- Dubinin N E, Yuryev A A and Vatolin N A 1998 *Thermochim. Acta* **316** 123
- Ducastelle F 1970 *J. Physique* **31** 1055
- Friedel J 1969 *The Physics of Metals* ed J M Ziman (New York: Cambridge University Press)
- Hafner J 1987 *From Hamiltonians to Phase Diagrams—The Electronic and Statistical–Mechanical Theory of s, p Bonded Metals and Alloys (Solid State Ser. vol 70)* (Berlin: Springer)
- Harrison W A and Froyen S 1980 *Phys. Rev. B* **21** 3214
- Hausleitner C and Hafner J 1988 *J. Phys. F: Met. Phys.* **18** 1025
- Hausleitner C, Kahl G and Hafner J 1991 *J. Phys.: Condens. Matter* **3** 1589
- Hultgren R R, Orr R L, Anderson P D and Kelley K K 1973 *Selected Values of Thermodynamic Properties of Metals and Alloys* (New York: Wiley)
- Jakse N and Bretonnet J L 1995 *J. Phys.: Condens. Matter* **7** 3803
- Jakse N, Wax J F, Bretonnet J L and Pasturel A 1996 *J. Non-Cryst. Solids* **205–207** 434
- Mackintosh A R and Andersen O K 1979 *Electrons at the Fermi Surface* ed M Springford (Cambridge: Cambridge University Press)
- Mansoori G A and Canfield F B 1969 *J. Chem. Phys.* **51** 4958
- Oli B A 1988 *IL Nuovo Cimento D* **10** 891
- Pines D and Nozières P 1966 *The Theory of Quantum Liquids* (New York: Benjamin)
- Regnaut C 1989 *Z. Phys. B* **76** 179
- Singh R N 1980 *J. Phys. F: Met. Phys.* **10** 1411
- Swan P 1967 *Nucl. Phys. A* **90** 436
- Umar I H, Meyer A, Watabe M and Young W H 1974 *J. Phys. F: Met. Phys.* **4** 1691
- Vashishta P and Singwi K 1972 *Phys. Rev. B* **6** 875
- Waseda Y 1981 *The Structure of Non-Crystalline Materials—Liquids and Amorphous Solids* (New York: McGraw-Hill)
- Weeks J D, Chandler D and Andersen H C 1971 *J. Chem. Phys.* **54** 5237
- Wills J M and Harrison W A 1983 *Phys. Rev. B* **28** 4363
- Yuryev A A 1985 *PhD Thesis* (Sverdlovsk: IMET UB RAS)
- Zerah G and Hansen J P 1986 *J. Chem. Phys.* **84** 2336