Integral thermodynamic properties of Mo and W in the nonempirical effective-potential approach

Genady Davidov and David Fuks
Materials Engineering Department, Ben-Gurion University of the Negev, Beer Sheva, Israel

Simon Dorfman
Department of Physics, Technion–Israel Institute of Technology, 32000 Haifa, Israel
(Received 11 July 1994; revised manuscript received 26 October 1994)

Cohesive and vibrational properties of W and Mo are calculated nonempirically. Parameters of a model are obtained by fitting to the equation of state (pressure-volume dependence). Partial and total densities of states are investigated for different pressures. It is shown that our method of fitting gives a good agreement of cohesive properties with the data calculated from the universal function of Rose *et al.* The applicability of the atomic-sphere approximation to the calculation of the integral thermodynamic properties of Mo and W is discussed.

I. INTRODUCTION

Molybdenum and tungsten are the refractory metals with a large cohesive energy and bulk modulus. Such properties cause wide use of these metals in the industry and are the topic of a lot of investigations in material science. Measuring of high-pressure properties of these metals (especially of tungsten) is a serious problem because of there extremely low compressibility. That is why any predictions of behavior of Mo and W in extremal conditions have to be appreciated. The progress in the electronic theory allows us now to produce quantitative predictions of the simple crystal structures of elements and some binary and ternary compounds by calculating the ground state energy of these systems. Recent developments in understanding the structural stability are achieved with the calculations at the absolute zero temperature. The rapid progress in the first-principles study of phases at nonzero temperatures may be obtained on the basis of modern first-principles approaches.[1] Using self-consistent band structure calculations, one can evaluate the binding energy curves for a system of atoms on a given lattice.[2,3] Analysis of such curves for elements and for simple compounds and alloys yields theoretical ground state properties such as cohesive energies, equilibrium lattice separations, bulk moduli, etc., that are in a good agreement with experimental data.[3–6] The nonempirical calculations of tungsten were used to study the influence of microalloying on the ductile-brittle phase transformation in W.[7–9]

Here, we present a straightforward procedure of evaluating different properties of W and Mo on the basis of nonempirical effective-potential approach. We shall base our calculations on the linear muffin-tin orbitals (LMTO) approach for solids.[10] The LMTO procedure is known to be a very effective method for nonempirical calculations of band structures. Recently, we used this method for calculations of the effective pair potentials for Cs (Ref. 11) and for description of the curved Arhenius plots in self-diffusion.[12] In this paper, we present the results of the first-principles LMTO-ASA (atomic-sphere approximation) calculations of electronic properties together with thermal properties of Mo and W. We discuss the limits of LMTO-ASA application to the pressure-volume diagram of these metals and show the way to overcome these limitations. Also, we give a scheme for prediction of the pressure-volume dependence in a wide region of volumes per atom (i.e., for highly compressed and highly tensed crystalline lattice). On the basis of the effective-potential approach, we calculate the cohesive energy as a function of volume and values of the second and fourth moments of phonon frequencies. These results are used for the calculation of the Debye temperature of Mo and W.

II. FORMALISM

Herewith we give the brief description of the theory which will be applied to the calculations. Self-consistent band structure calculations for the set of the cell volumes, Ω, give the volume dependence of the total energy, $E_{\rm tot}$, of the crystal:

$$E_{\rm tot} = E(\Omega). \tag{1}$$

In order to perform self-consistent field calculations in the ASA, the spherically averaged electronic density is used, and for this purpose the one-center expansions are sufficiently accurate. The total energy of the electrons in the ground state may, according to density-functional theory,[3] be estimated as

$$E_{\rm tot} = \sum^{\rm occ} \epsilon_i - E_{\rm dc} + E_{\rm el} + E_{\rm ec}. \tag{2}$$

Here, ϵ_i are the one-electron terms, $E_{\rm dc}$ is the double counting energy, $E_{\rm el}$ is the electrostatic energy which can be calculated from the Madelung constants, and $E_{\rm ec}$ is the exchange-correlation energy. $E_{\rm dc}$ is calculated from the electronic density, $\rho(r)$ and crystal potential, $V(r)$, as

$$E_{dc} = \frac{1}{2}\int \rho(r)V(r)dr. \tag{3}$$

Here, $V(r)$ is a spherically symmetric potential. It is now fairly simple using the Born-Oppenheimer and the local-density-functional approximations[2] to carry out first-

principles calculations of the full pressure[6] at zero temperature, that is the change of the total energy with uniform compression, i.e.,

$$P(\Omega) = -\frac{dE_{\rm tot}}{d\Omega}. \tag{4}$$

We have neglected in Eq. (4) the zero-point motion of the nuclei. Performing these calculations on a large set of volumes, we receive the dependence of the pressure on the volume, which enables us to estimate the equilibrium atomic volume, Ω_0, from the condition

$$P(\Omega_0) = 0. \tag{5}$$

From this dependence the bulk modulus, or inverse compressibility, B,

$$B = -\left[\frac{dP}{dln\Omega}\right]_{\Omega=\Omega_0}, \tag{6}$$

and the cohesive energy, $E_{\rm coh}$,

$$E_{\rm coh} = -\int_{\Omega_0} P d\Omega, \tag{7}$$

may be obtained. We want to emphasize that it is possible to perform calculations of the full pressure with the same accuracy as calculations of the potential parameters in the LMTO scheme.[13] On the other hand, the total energy may be expressed as the sum of effective pair potentials,

$$E_{\rm tot} = \frac{1}{2}\sum_{i,j;i\neq j} \Phi(|\vec{r_i} - \vec{r_j}|). \tag{8}$$

The double summation here is done over all atom positions. In further calculations, we will use Morse-type pair potentials:

$$\Phi(r) = D\exp[-2\lambda(r - r_0)] - 2D\exp[-\lambda(r - r_0)]. \tag{9}$$

The choice of this form of potentials is dictated by the results obtained in the framework of embedded atom method (EAM) approach. This method was introduced in Refs. 14 and 15 and widely used for description of different properties of metals, especially for Mo and W.[16,17] The effective potentials obtained in Refs. 18–20 from EAM are very close to the Morse potential form. These effective potentials give only a part of the total energy, whereas the Morse potential is intended to provide the $E_{\rm tot}$.

It is well known that pair potential approach is absolutely inapplicable for the investigation of elastic properties of metals. The main reason is the validity of the Cauchy relation, $C_{12} = C_{44}$, which is the direct consequence following from the pair potential approximation. This relation is not true for most of metals. However, if we are interested in cohesive properties, they may be reasonably described by the Morse pair potential approximation. We will compare our results with the Ref. 21, where the cohesive energy of most metals as a function of lattice constant was scaled to a simple universal function,

$$E(a) = -E_{\rm coh}(1 + a^*)\exp(-a^*). \tag{10}$$

In this expression, $E_{\rm coh}$ is the absolute value of the cohesion energy at zero temperature and pressure. The quantity a^* is a measure of the deviation from the equilibrium lattice constant,

$$a^* = (a/a_0 - 1)/(E_{\rm coh}/9B\Omega_0)^{\frac{1}{2}}. \tag{11}$$

a is a length scale characteristic of the condensed phase, which we will take to be the lattice constant, and a_0 is the equilibrium lattice constant. The parameters of potential (9) will be obtained by fitting to the pressure-volume dependence carried out from LMTO-ASA calculations for different volumes. Making use of this potential, we obtain the second moment of frequency spectrum $\overline{\omega^2}$,

$$\overline{\omega^2} = \frac{1}{3sN}\sum_{\vec{k},j}\omega^2(\vec{k}) = \int_0^{\omega_m}\omega^2 g(\omega)d\omega. \tag{12}$$

s is the number of atoms per unit cell, j is the number of the phonon frequency branches, ω_m is the maximum frequency in the phonon spectrum, and $g(\omega)$ is the density of states. The quantity $\overline{\omega^2}$ is defined by the trace of dynamic matrix. For solids with one atom per primitive cell, $\overline{\omega^2}$ is related with force constants by[22]

$$\overline{\omega^2} = \frac{1}{3M}\sum_{l,\alpha}{}' F_{\alpha\alpha}(l). \tag{13}$$

The prime shows exclusion of the term with $l = 0$. In Eq. (13), M is the atomic mass, $F_{\alpha\beta}$ are force constants determining the dynamic matrix. These constants may be expressed in the pair potential approximation as follows:

$$-F_{\alpha\beta} = x_\alpha x_\beta\left(\frac{\Phi''}{r^2} - \frac{\Phi'}{r^3}\right)_{r=R_l} + \delta\left(\frac{\Phi'}{r}\right)_{r=R_l}. \tag{14}$$

l represents three numbers, showing the position of the lattice site, x_α and x_β are the projections of the lattice vector $\vec{R}_l$ on the corresponding axis, Φ' and Φ'' are the first and second derivatives of the effective pair potentials with respect to r, and δ represents the terms of the higher order in $\left(\frac{\Phi'}{r}\right)_{r=R_l}$. Hence, the second moment of phonon spectrum may be expressed in the terms of force constants and may be obtained without direct calculations of phonon spectrum and density of states by means of

$$\overline{\omega^2} = \frac{1}{3M}\sum_i z_i\left(2\frac{\Phi'}{r} + \Phi''\right)_{r=R_i}. \tag{15}$$

In Eq. (15), z_i is the number of neighbors in the ith shell.

The second moment $\overline{\omega^2}$ is related to the Debye temperature in the high-temperature limit by a simple expression[23]

$$\Theta_D^\infty = \lim_{T\to\infty}\Theta_D = [5\hbar^2\overline{\omega^2}/(3k^2)]^{\frac{1}{2}}. \tag{16}$$

Θ_D^∞ is the high-temperature limit of the Debye temperature as determined from specific heat measurements.

This expression is frequently used as the experimental value of Θ_D, quoted without further comments in the literature for a given substance (see for example Ref. 24).

In order to investigate the temperature dependence of Debye temperature in the high-temperature region, we will use the expansion, given in Refs. 23 and 25,

$$\Theta_D^2 = [\Theta_D^\infty]^2 \left\{ 1 - \frac{3}{100} \left[\frac{\Theta_D^\infty}{T} \right]^2 \left(\frac{\overline{\omega^4}}{\overline{\omega^2}^2} - \frac{25}{21} \right) + \cdots \right\}. \tag{17}$$

The fourth moment of the phonon spectrum, $\overline{\omega^4}$ may be also expressed in terms of force constants,

$$\overline{\omega^4} = (\overline{\omega^2})^2 + \frac{1}{3M^2} \left(\sum_{l,\alpha}{}' (F_{\alpha\alpha}(l))^2 + \sum_{l,\alpha\neq\beta} (F_{\alpha\beta}(l))^2 \right). \tag{18}$$

Thus, carrying out calculations according to the Eq. (14) and making use of $\overline{\omega^2}$ and $\overline{\omega^4}$ according to the Eqs. (15) and (18), we may get the temperature dependence of the Debye temperature from the first principles. Further we will perform these calculations and compare the results with the experimental values.

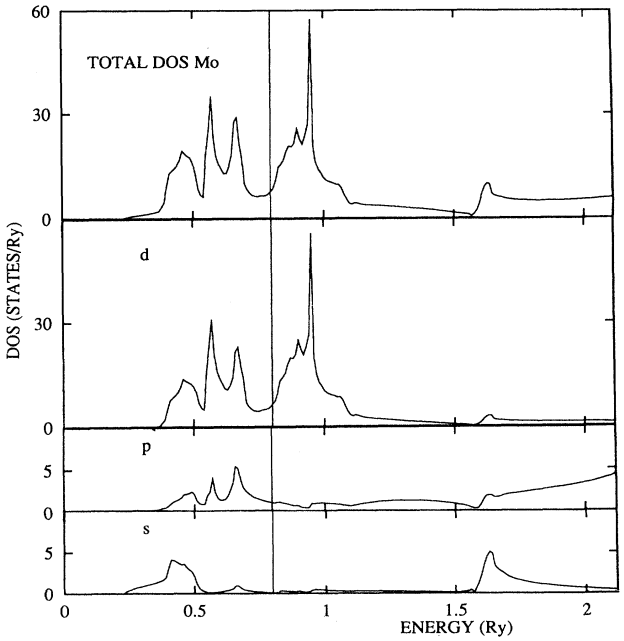

FIG. 1. The total and partial DOS of bcc Mo.

III. RESULTS AND DISCUSSION

Our first-principles calculations of the equation of states at zero temperature, i.e., the change in the total energy, $E_{\rm tot}$, with uniform compression, were carried out. The self-consistent crystal potentials for bcc W and Mo were generated in LMTO-ASA band structure calculations. We included also the relativistic corrections in the scalar-relativistic scheme (without the spin-orbit coupling). Calculations have been performed for set of different lattice parameters, on the mesh corresponding to 285 $\vec{k}$ points in the irreducible wedge of the Brillouin zone. The integration has been done by the tetrahedron method and the Gunnarson-Lundquist exchange-correlation potential in the local-density approximation was used.[26] We found band structures that are practically identical with the results of the previous papers.[27] The total and partial density of states (DOS) for Mo are presented in Fig. 1. It is easy to see that the main contribution to the total DOS at high energy is given by the p electrons, while in the neighborhood of the Fermi level the d electrons, as well known, are playing the main role. Up to the energy 1.6 Ry our DOS are in good agreement with the results of Ref. 27. Figure 2 shows the DOS of W for different pressures. Increasing of the pressure leads to decreasing of the height of picks with the broadening of them in DOS. Figure 3 represents changes of s-, p-, and d-partial contributions and the total DOS at the Fermi level.

We would like to emphasize that quality of the obtained values of the pressure are of the same order of accuracy as a quality of the band structure calculations in the framework of the LMTO-ASA approach.[13] At the same time, the results of $E_{\rm tot}$ calculations in this scheme are much less accurate. From our calculations on a large set of volumes, we extract the equilibrium volume Ω_0 at $P = 0$ for Mo and W. The carried out lattice parameters are $a_{\rm Mo} = 6.05$ a.u. and $a_{\rm W} = 6.06$ a.u. These values are in good agreement with the experimental results ($a_{\rm Mo} = 5.89$ a.u., $a_{\rm W} = 5.98$ a.u.).[28]

In the region of positive pressures (see Fig. 4), we compare our results with experimental data[29] for Mo. Our curve is higher in comparison with the measured values because the bulk modulus obtained in the LMTO-ASA approximation is also higher than the experimental ones (see Table I). The analogous curve for tungsten is given on Fig. 5 and may be of special interest as a prediction of the equation of state for W. Unfortunately, to the best of our knowledge, the experimental data for W is absent. This is because of extremely high values of bulk modulus, the highest among all metals. Nevertheless we have compared our results with the universal function of Rose *et al.*[21]

We have calculated the pressure-volume dependence for W for a wide region of volumes, in such a way simulating the positive and negative pressures (compressed and tensiled states). The results of our LMTO-ASA calculations are given in the Fig. 6 (solid curve). If now we will try to use Eq. (7) for calculations of the cohesive energy, the very large value of it will be obtained. That means that one may apply the LMTO-ASA only in a narrow region near the equilibrium volume Ω_0. In order to overcome this difficulty, we will use the LMTO-ASA method together with the pair potential approximation for the description of the cohesive energy. Making use of Eqs. (4), (8), and (9), the following expression for the pressure in terms of pair potentials may be obtained,

$$P = \frac{-2\lambda D}{3a^3} \sum_{i=1}^{N} z_i R_i \{\exp[\lambda\ (R_i - r_0)] - \exp[-2\lambda(R_i - r_0)]\}. \quad (19)$$

The summation is performed over coordination shells, i, with the radius R_i up to Nth shell and z_i is the number of atoms in the ith shell. Now we have several possibilities to define the parameters of the effective pair potential: (1) by solving the system of equations in numbers equal to the number, n, of potential parameters for given values $P(\Omega_1)$, $P(\Omega_2)$, ..., $P(\Omega_n)$; (2) by fitting the potential parameters in the overfilled system of equations for a lot of values $P(\Omega_k)$. Such a fitting has to be done on a large set of volumes near equilibrium.

We choose the second way and obtained the pair potential parameters, given in Table II. We produced the summation in Eq. (19) up to 8th shell. The changes of the cohesive energy Eq. (8) do not exceed 0.01 eV when the ninth shell is included in Eq. (19). The fitted parameters of potentials only slightly deviate from the parameters of the Morse potentials computed from experimental data.[30] In Ref. 30, Girifalco and Weizer applied a Morse-type potential to cubic metals by computing the potential parameters from basic crystal properties: cohesive energy, equilibrium lattice parameter, and bulk modulus. The value of cohesive energy was compared in Ref. 30 with experimental energy of sublimation extrapolated to zero temperature and pressure. Making use of our pair potentials, we calculated the modified pressure-volume dependence for tungsten (dotted curve in Fig. 6). This

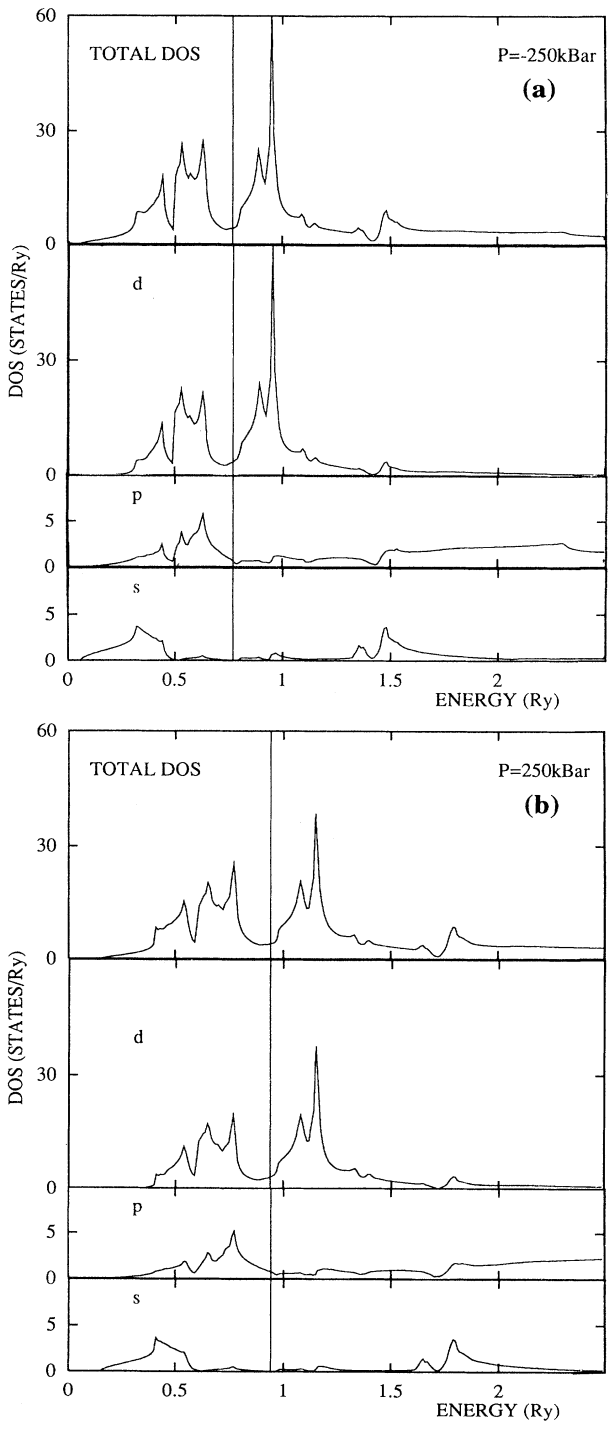

FIG. 2. The total and partial DOS of bcc W for different pressures.

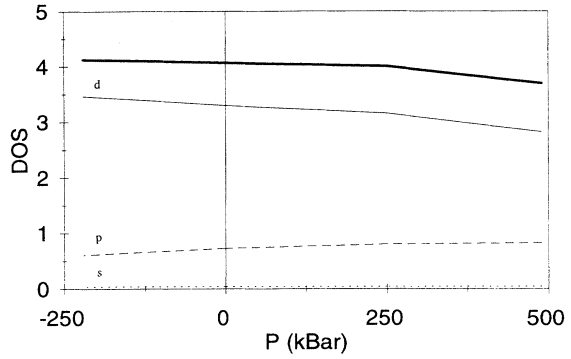

FIG. 3. The dependences of s-, p-, d- partial DOS and the total DOS (solid curve) on the Fermi level on the pressure for W.

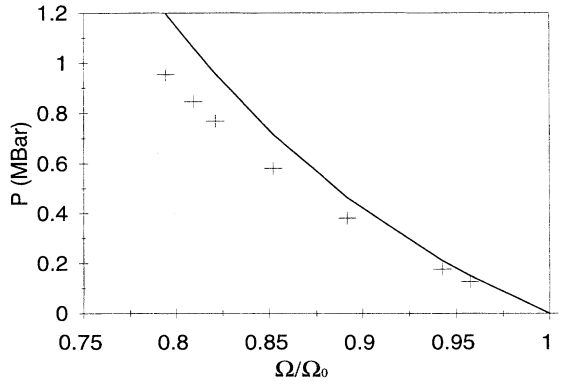

FIG. 4. The dependence of pressure on atomic volume for Mo. The solid curve represents the LMTO-ASA calculations and the markers are corresponding to the experimental results (Ref. 29).

TABLE I. Properties of metals calculated in the framework of LMTO-ASA (the top value represents the calculated value, and the bottom value is the experimental data).

	W	Mo
a_0 (a.u.)	6.06	6.05
	5.98[a]	5.89[a]
B (GPa)	350	300
	311[b]	261[b]
E_{coh} (eV)	9.3	7.3

[a]Reference 28.
[b]Reference 31.

dotted curve gives a much smaller value of cohesive energy, in comparison with that obtained directly by means of $P(\Omega)$ dependence in LMTO-ASA calculations. Using our pair potentials, we found the volume dependence of cohesive energy (Fig. 7) and the equilibrium cohesive energy. The results for Mo and W are given in Table I, together with the experimental data. As shown in Fig. 7, our results are in excellent agreement with the universal function (10) of Rose *et al.*[21] Both Figs. 5 and 7 show the quality of our calculations of the cohesive properties of W. Not only the cohesive energy, but also it's derivative with respect to volume is well defined, thus encouraging us to calculate the vibrational properties of tungsten. We would like to emphasize that our parameters for pair potential were obtained by fitting to the pressure-volume dependence. These potentials are representing the curvature of $E_{coh}(\Omega)$ in a more proper way in comparison with the simple direct fitting to the universal function $E_{coh}(\Omega)$ of Rose *et al.*[21] Such an agreement of E_{coh} with experimental data gives a possibility to estimate the limits of applicability of LMTO-ASA calculations for the investigated metals. Figure 6 shows that, for example, for W, the 15% deviations of volume near the equilibrium value gives a reasonable accuracy for the LMTO-ASA method to reproduce the cohesive energy. Potentials for W and Mo were used for calculations of the second and

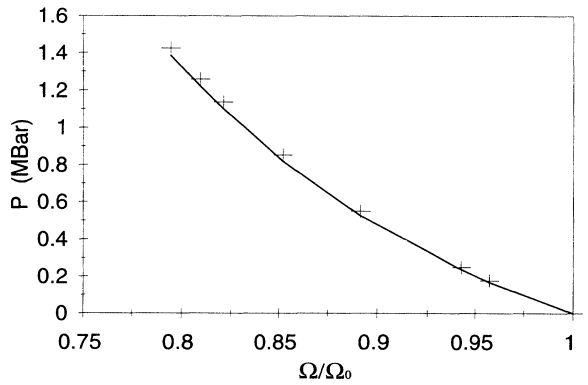

FIG. 5. The dependence of the pressure on the atomic volume for W. The markers are showing the data of LMTO-ASA calculations. The solid curve is the universal curve of Rose *et al.* (Ref. 21).

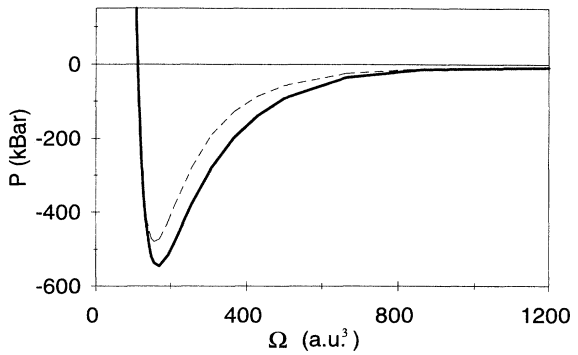

FIG. 6. Pressure-volume diagram for W for a large region of volumes by LMTO-ASA calculations (the solid curve) and a modified dependence (shown by the dotted line).

TABLE II. Parameters of Morse pair potential fitted within the suggested procedure (the top value represents the calculated value, and the bottom value were computed in Ref. 30 from experimental data).

	W	Mo
D (eV)	1.1	0.9
	1.0	0.8
λ (a.u.$^{-1}$)	0.775	0.8
	0.747	0.8
r_0 (a.u.)	5.74	5.70
	5.73	5.63

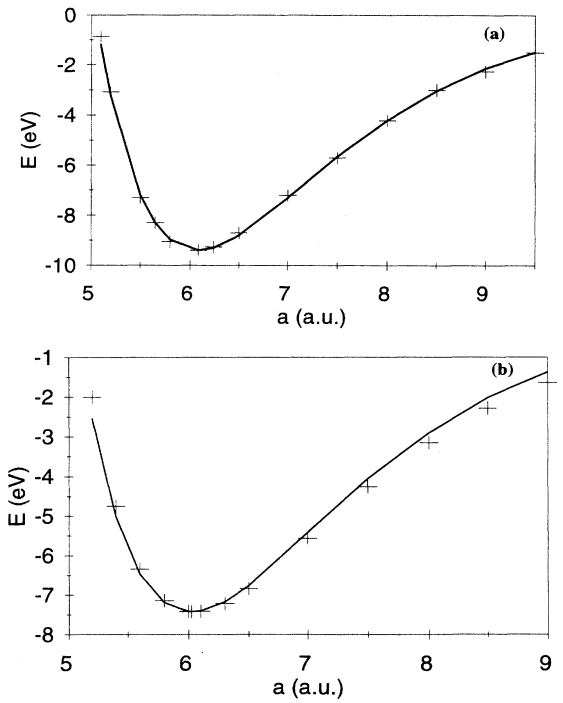

FIG. 7. The cohesive energy as a function of a lattice parameter for W (a) and Mo (b). The solid line is the universal curve of Rose *et al.* (Ref. 21), the markers are the results of our calculations.

TABLE III. The coordination shell's contributions to the second moment of the phonon spectra for W and Mo.

Number of the shell	The terms of sum in Eq. (15) W	Mo
1	1.564	1.457
2	0.242	0.213
3	-0.055	-0.048
4	-0.047	-0.039
5	-0.011	-0.010
6	-0.003	-0.002
7	-0.005	-0.004
8	-0.004	-0.003

the fourth moments of phonon spectrum with expressions (15) and (18). The results for $\overline{\omega^2}$ are given in Table III. We studied the convergency of Eq. (15) and as it is seen from the Table II, the main contribution to $\overline{\omega^2}$ is given by the first shell (more than 90% for both of the elements). The Debye temperatures at different conditions $T \to \infty$ and $T = 298$, Θ_D^{∞} and Θ_D^{298}, respectively, were calculated with Eqs. (16) and (17) and are presented in Table IV together with the experimental data.[24] In real crystals, the Debye temperature varies upon the temperature and is different for different properties. $\Theta_D^{\exp}$ refers to the Debye temperature at 298 K. It was previously calculated for metals in Ref. 24 from the measurements of specific heat at constant volume. Extended data are also given in Ref. 32. We would like to mention that the values of Θ_D^{298} obtained from elastic constants measurements and given in Ref. 32 are equal to 370 K for W and 454 K for Mo. However, we find it expedient to compare our results with the Θ_D^{298} obtained from the specific heat measurements,[24,32] because as noted in Ref. 33, the value of Θ_D calculated from theoretical relations (16), (17) equivalent to the Debye temperature determined from this type of measurements. The whole subject and how to relate various moments of the frequency distribution to thermal data is discussed by Barron *et al.* in a series of papers (see, for example, Refs. 25 and 34).

It is usually considered and is a well-known fact that the dispersion law calculated in the framework of pair potential approach will come out wrong. Nevetheless, we showed here that such potentials, if they are determined by the described procedure, may be successfully applied to the calculations of integral spectral characteristics such as $\overline{\omega^2}$ and Θ_D. Especially in these cases, it follows that it is not necessary to reproduce the details of the phonon spectrum, and the obtained data are well correlated with the results of measurements.

TABLE IV. The second and fourth momenta of the phonon spectra ($\overline{w^2}$ and $\overline{w^4}$) and the Debye temperature, Θ_D, for W and Mo. $\Theta_D^{\exp}$ refers to the Debye temperature at 298 K obtained in Ref. 24 from the specific heat data.

	W	Mo
$\overline{w^2}(10^{-27}\ \mathrm{sec}^2)$	1.697	1.564
$\overline{w^4}(10^{-54}\ \mathrm{sec}^4)$	6.490	5.176
Θ_D^{∞}, K	404	390
Θ_D^{298}, K	392	380
$\Theta_D^{\exp}, K$	310	380

IV. SUMMARY

We presented here the results of first principles LMTO-ASA calculations for bcc Mo and W. In order to obtain realistic values of cohesive energy and its volume dependence, we suggested a scheme that allows us to get from the pressure-volume dependence, the parameters of effective pair potentials, and the cohesive energy. The last is of great importance, because in the framework of LMTO-ASA, the pressure is usually calculated with just the same accuracy as the band structure.[13] The densities of states (total and partial for Mo and W) were calculated as the functions of pressure. In the region (−250–500 kBar), the decreasing of the value $N(E_f)$ is obtained when the pressure increases. On the basis of the carried out equation of states, we calculated the equilibrium lattice parameter and the compressibility. We got the parameters of effective pair potentials by fitting to equation of states. These potentials were used further to determine the cohesive energy, second and fourth momenta of phonon spectra, and the Debye temperature for Mo and W. The data on the cohesive energy calculations were compared with the universal function of Rose *et al.*[21] and showed very good agreement. We also discussed the convergency of the direct calculations of $\overline{\omega^2}$ and the Debye temperature for Mo and W on the basis of an effective pair potential approach and showed that the series are rapidly converged. The results of our calculations eliminate additional possibilites and limits in applicability of LMTO-ASA calculations for the elements under investigation.

ACKNOWLEDGMENTS

This work was supported in part by Israel Ministry of Science, Grant Nos. 3616 and 4868 and by Israel Ministry of Absorbtion under the special program for the science adsorbtion. One of us (D.F.) is thankful to the Rashi Foundation for support. The support of the Niedersäehsischen Ministeriums für Wissenschaft und Kultur is appreciated.

[1] K. Binder, Mater. Sci. Technol. Encycl. **5** (1992).
[2] W. Kohn, *Highlights of Condensed-Matter Theory*, edited by F. Bassani, F. Fumi, and M.P. Tosi (North-Holland, Amsterdam, 1985), p. 1.
[3] H.L. Skriver, Phys. Rev. B **31**, 1909 (1985).
[4] V.L. Moruzzi, J.F. Janak, and K. Schwarz, Phys. Rev. B **37**, 790 (1988).
[5] J.M. Sanchez, J.P. Stark, and V.L. Moruzzi, Phys. Rev. B **44**, 5411 (1991).
[6] D.G. Pettifor, Commun. Phys. **1**, 141 (1976).
[7] G.L. Krasko, Scr. Met. Mater. **28**, 1543 (1993).
[8] G. L. Krasko (unpublished).

[9]G.L. Krasko and G.B. Olson, Solid State Commun. **76**, 247 (1990); **79**, 113 (1991).
[10]H.L. Skriver, *The LMTO Method* (Springer, New York, 1984).
[11]S. Dorfman and D. Fuks, Z. Phys. B **91**, 225 (1993).
[12]D. Fuks, J. Pelleg, S. Dorfman, and S. Rashkeev, Solid State Commun. **87**, 405 (1993).
[13]D.G. Pettifor, J. Phys. F **8**, 219 (1978).
[14]M.S. Daw, S.M. Foiles, and M.I. Baskes, Mater. Sci. Rep. **9**, 251 (1993).
[15]M.S. Daw and M.I. Baskes, Phys. Rev. B **29**, 6443 (1984); M.S. Daw, *ibid.* **39**, 7441 (1989), and references therein.
[16]M.W. Finnis and J.E. Sinclair, Philos. Mag. A **50**, 45 (1984).
[17]R.A. Johnson and D.J. Oh, J. Mater. Res. **4**, 1195 (1989).
[18]J.B. Adams and S.M. Foiles, Phys. Rev. B **41**, 3316 (1990).
[19]S.P. Chen, D.J. Srolovitz, and A.F. Voter, J. Mater. Res. **4**, 62 (1989).
[20]R.A. Johnson, Phys. Rev. B **37**, 3924 (1988).
[21]J.H. Rose, J.R. Smith, F. Guinea, and J. Ferrante, Phys. Rev. B **29**, 2963 (1984).
[22]G. Leibfried, *Encyclopedia of Physics* (Springer, Berlin, 1955), Vol. 7, Pt. 1, p. 104.
[23]C. Domb and L. Salter, Philos. Mag. **43**, 1083 (1952).
[24]J. de Launay, in *Solid State Physics: Advances in Research and Applications*, edited by F. Seitz and D. Turnbull (Academic, New York, 1956), Vol. 2, p. 219.
[25]T.H.K. Barron, W.T. Berg and J.A. Morrison, Proc. R. Soc. London Ser. A **242**, 478 (1957).
[26]L. Hedin and B.I. Lundquist, J. Phys. C **4**, 2064 (1971).
[27]D.A. Papaconstantopoulos, *Handbook of the Band Structure of Elemental Solids* (Plenum, New York, 1986).
[28]*Smithells Metals Reference Book*, 6th ed. (Butterworths, London, 1983), Vol. 1.
[29]H.K. Mao, P.M. Bell, J.W. Shaner, and D.J. Steinberg, J. Appl. Phys. **49**, 6 (1978).
[30]L.A. Girifalko and V.G. Weizer, Phys. Rev. **114**, 687 (1959).
[31]C. Kittel, *Introduction to Solid State Physics*, 5th ed. (Wiley, New York, 1976).
[32]A. Karl and Jr. Gschneidner, in *Solid State Physics: Advances in Research and Applications*, edited by F. Seitz and D. Turnbull (Academic, New York, 1964), Vol. 16, p. 368.
[33]L. Salter, Proc. R. Soc. London Ser. A **233**, 418 (1955).
[34]T.H.K. Barron and M.L. Klein, in *Dynamical Properties of Solids*, edited by G.K. Horton and A.A. Maradudin (North-Holland, Amsterdam, 1974), Vol. 1, p. 391.