PHYSICAL REVIEW B
CONDENSED MATTER

THIRD SERIES, VOLUME 50, NUMBER 11 15 SEPTEMBER 1994-I

Calculations of the total energy, electron-phonon interaction, and Stoner parameter for metals

M. M. Sigalas
Ames Laboratory, Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011

D. A. Papaconstantopoulos
Complex Systems Theory Branch, Naval Research Laboratory, Washington, D.C. 20375-5345

(Received 7 April 1994)

Using the augmented-plane-wave method, we performed total-energy calculations for all the metals crystallizing in the hcp structure and for all the 5*d* metals in the hcp structure. Also, using the predicted equilibrium lattice constants from our present and previous total-energy calculations, we carried out band-structure calculations that explore possibilities for superconductivity and magnetism in all the transition metals in the fcc, bcc, and hcp structures.

I. INTRODUCTION

In the first part of this paper (Sec. II) we present calculated values of the equilibrium lattice constants and bulk moduli of all elements whose equilibrium structure is hcp and, in addition, of all the 5*d* metals in the hcp structure. The present calculations are a continuation of our previous work[1,2] in which we studied the alkali metals and the 3*d*, 4*d*, and 5*d* metals in both fcc and bcc structures. There are three basic motivations for this study. (1) Recently, Cortella *et al.*[3] found evidence of metastable phases for fcc Re and an *A* 15 form of Ta. Interestingly, the experimental measurements of their melting temperatures are in good agreement with theoretical results based on total-energy calculations similar to those presented here. In that sense, the total-energy differences between the various structures may be used as a guide for further experimental observations of metastable phases of other metals. (2) Our previous total-energy results[1] already have been used in order to find the parameters of tight-binding models,[4] so, the time consuming first-principles calculations in low-symmetry structures can be avoided. By including the present hcp results in the fitting procedure, we expect even better results from the tight-binding model. Also, the constant electron density in the intenstitial region of the muffin-tin potentials can be used for the calculations of the elastic properties of the metals by using the newly proposed ideal metal model.[5] (3) Finally, the present and previous[1] results can be used for the study of certain trends along each *d* series and their dependence on the structure.

In accordance with the third motivation, we study (Sec. III) the trends of the McMillan-Hopfield parameter[6] η and the magnetic properties[7] across each *d* series for all the calculated structures. The parameter η controls the electron-phonon interaction, which can be used to determine, at least semiquantitatively, the superconducting transition temperature.[6] The magnetic properties of the materials were calculated within the Vosko-Perdew theory[7] from which the susceptibility enhancement can be found and possible ferromagnetic instabilities can be predicted.[7]

II. TOTAL-ENERGY CALCULATIONS FOR hcp STRUCTURES

A. Method of calculation and approximations

The total energy was calculated from the expression of Janak,[8] which is valid within the muffin-tin (MT) approximation and needs the crystal potential, the charge density, and the eigenvalue sum as input. These were calculated self-consistently by the augmented-plane-wave (APW) method[9] in its general version using the MT approximation, which has been proven accurate for cubic materials,[1,2] we expect the same accuracy for hcp materials.

To determine the charge density and the potential self-consistently, we treated the highest *s* and *d* orbitals as band levels. All other states were treated as core levels because they form essentially flat bands. The core levels were calculated by a fully relativistic atomiclike calculation in each iteration. The band states were calculated self-consistently in the semirelativistic approximation[10] (the spin-orbit coupling is neglected) on a mesh of 45 **k** points in the irreducible Brillouin zone.

In all calculations, the exchange potential was treated in the exchange and correlation formalism of Hedin and Lundqvist.[11] To find the equilibrium lattice constants, we calculated the total energy at various lattice constants, and determined the minimum by fitting the results with a parabolic fit to both the inverse of the volume and the inverse of the c/a ratio, with rms fitting errors less than 0.5 mRy.

B. Results

Our results for the c/a ratio, the equilibrium volume, the bulk modulus, and the energy difference between hcp and fcc structures are presented in Table I. The agreement with experiment[12] is very good especially for the elements in the seventh (Tc,Re) and eighth (Ru,Os) columns; for those elements, the percentage differences are within 1.5 and 20% for the equilibrium volumes (V_o) and the bulk moduli (B_o), respectively. Those differences are higher for the elements in the second (Be,Mg), third (Sc,Y,La), and fourth (Ti,Zr,Hf) columns; they are within 8 and 43% for V_o and B_o, respectively. The present results for B_o of Sc and Ti are in very good agreement (less than 8% differences) with previous full-potential calculations,[13] while our calculated V_o for Sc and Ti are almost identical with those of Ref. 13. So, it seems that the relatively higher differences from experiment for those metals are not due to the muffin-tin approximation. Recent calculations[14] for transition metals show that the generalized-gradient approximation[15] corrects these differences for the alkali elements. But for transition metals, the results show improvement in most but not in all cases.[16] The c/a ratio is in excellent agreement with experiment for all the elements presented in Table I. However, for elements with c/a far from the ideal value of 1.633 (such as Zn and Cd), the muffin-tin approximation fails since it tends to find a minimum for the total energy close to the ideal value. The reason is probably the fact that for these metals one uses c/a values much higher than the ideal and the packing ratio becomes smaller than in the closed-packed structure.

The energy differences ΔE, between hcp and fcc structures always predict the correct structure ($\Delta E < 0$ for hcp and $\Delta E > 0$ for fcc). They are also in good agreement with previous calculations. Fernando *et al.*[17] calculated the values of ΔE for the $5d$ series (Hf-Au) using both the full potential and the muffin-tin version of the linear-augmented Slater-type orbital method. The present results for the $5d$ elements are in very good agreement with their full-potential results except for Os where they are closer to their muffin-tin results. In their muffin-tin version, they used a nontouching spheres approach—in contrast with our approach. In fact, Fernando *et al.*[17] stated in their paper that using touching spheres improves the agreement with their full-potential results. The ΔE's for Sc and Ti are also in good agreement with the full-potential linear muffin-tin orbitals results of Paxton, Methfessel, and Polatoglou.[13] Finally, our ΔE ($=-4.5$ mRy) for Re is in excellent agreement with the ΔE ($=-4.8$ mRy) calculated by Cortella *et al.*[3] Interestingly, they used that value as well as the experimental value of the enthalpy of melting of the hcp Re, in order to predict the melting temperature of the metastable fcc Re; the predicted temperature is in very good agreement with the measured temperature.[3] The experimental technique (high undercooling of refractory metals) used in Ref. 3 seems to be an exciting way to get metastable transformations and the present total-energy results for hcp structures as well as our previous results[1] for fcc and bcc structures can be used as a guide for searching candidate elements exhibiting these kinds of transformations.

The trends that we find for the relative stability of the crystal structures along the $5d$ series (we expect the same trends for $3d$ and $4d$ series) are consistent with experiment as also was found by Fernando *et al.*,[17] Skriver,[18]

TABLE I. c/a ratios for hcp structures, volume per atom (V_o), equilibrium bulk moduli (B_o), and the total-energy differences (ΔE) between hcp and fcc structures.

Element	c/a Theor.	c/a Expt.	V_o (a.u.) Theor.	V_o (a.u.) Expt.	B_o (MBar) Theor.	B_o (MBar) Expt.	ΔE (mRy)
Be	1.590	1.581	50.50	54.06	1.441	1.003	−4.0
Mg	1.637	1.623	144.30	156.87	0.394	0.354	−0.4
Sc	1.560	1.592	150.60	168.72	0.647	0.435	−2.5
Ti	1.616	1.586	108.60	119.01	1.290	1.051	−2.1
Y	1.594	1.570	203.00	223.07	0.483	0.366	−0.3
Zr	1.620	1.594	151.40	157.00	1.192	0.833	−1.4
Tc	1.616	1.606	95.80	96.53	3.637	2.970	−4.4
Ru	1.612	1.579	91.00	91.87	3.573	3.208	−4.6
		$5d$ metals					
Ba	1.606		382.40		0.146		0.3
La	1.662	1.619	257.20	249.48	0.495	0.243	−3.3
Hf	1.620	1.583	152.00	150.17	1.188	1.090	−4.6
Ta	1.662		123.20		2.206		4.2
W	1.672		110.20		3.208		9.4
Re	1.624	1.616	100.76	99.28	3.879	3.720	−4.5
Os	1.610	1.577	95.26	94.77	4.307	4.180	−3.6
Ir	1.634		97.30		3.591		11.2
Pt	1.666		103.90		2.412		10.3
Au	1.647		115.10		2.068		1.9

and Paxton, Methfessel, and Polatoglou.[13] This trend is an hcp→bcc→hcp→fcc sequence as the d bands become progressively filled. This was explained semiquantitatively by Pettifor[19] more than 20 years ago by using a model characterized by only two d-resonance parameters from which the densities of states were obtained in a hybrid nearly free electron and tight-binding scheme.

Finally, our present and previous[1] results for the alkaline-earth metals agree with the experimental observations for the equilibrium structures and the small energy differences between the different structures suggest possible structural changes in accordance with experiment and previous theoretical work (see Ref. 18).

III. ELECTRON-PHONON INTERACTION AND STONER PARAMETER

A. Theory

The electron-phonon coupling constant is given by the McMillan formula

$$\lambda=\frac{\eta}{M\bar{\omega}^2}\,, \tag{1}$$

where the force constants $M\bar{\omega}^2$ can be found from neutron-scattering data or frozen phonon calculations, and the McMillan-Hopfield parameter η is determined using the "rigid muffin-tin" approximation developed by Gaspari and Gyorffy[6] and is given by

$$\begin{aligned}\eta&=N(E_F)\langle I^2\rangle\\&=\frac{E_F}{\pi^2 N(E_F)}\sum_{\ell}2(\ell+1)\sin^2(\delta_{\ell+1}-\delta_{\ell}\frac{N_{\ell}N_{\ell+1}}{N_{\ell}^{(1)}N_{\ell+1}^{(1)}}\,,\end{aligned} \tag{2}$$

where δ_{ℓ} is the scattering phase shift at the Fermi energy E_F and the angular momentum ℓ, $N_{\ell}^{(1)}$ is the single-scatterer density of states (DOS) defined in Ref. 6. N_{ℓ} and $N(E_{F)}$ are the ℓ partial and total DOS, respectively, at E_F. Equation (2) is exact to $\ell=1$, but for higher values of ℓ it involves nonspherical corrections. However, for the hcp materials such corrections are expected to be very small.

The necessary input to Eq. (2) was generated as follows: (a) the phase shifts δ_{ℓ} were found from the logarithmic derivatives of the radial wave functions that correspond to the self-consistent crystal potentials of each element, (b) the DOS $N(E_F)$ and N_{ℓ} were computed by the tetrahedron method,[20] and (c) the free scatterers $N_{\ell}^{(1)}$ were calculated using the radial wave functions of the above crystal potentials.

TABLE II. Electron-phonon interaction and Stoner criterion parameters for 3d metals.

System	$N(E_F)$ (Ry^{-1}/atom/spin)	I_F (Ry)	$I_F N(E_F)$	η (eV/Å^2)	$\langle I^2\rangle$ (Ry/a.u.)^2
Ca bcc	4.620	0.0180	0.1668	0.1885	0.000 840
Ca fcc	4.389	0.0186	0.1634	0.1507	0.000 706
Sc bcc	16.515	0.0181	0.5980	3.4515	0.004 301
Sc fcc	12.280	0.0202	0.4968	2.8481	0.004 773
Sc hcp	14.733	0.0198	0.5834	2.6362	0.003 682
Ti bcc	11.642	0.0197	0.4594	6.3085	0.011 152
Ti fcc	12.533	0.0213	0.5331	6.1358	0.010 075
Ti hcp	6.302	0.0210	0.2653	2.7509	0.008 983
V bcc	13.737	0.0218	0.5989	10.5133	0.015 750
V fcc	10.099	0.0231	0.4675	6.2220	0.012 679
Cr bcc	4.782	0.0244	0.2338	4.2893	0.018 459
Cr fcc	11.372	0.0256	0.5831	6.8674	0.012 428
Mn bcc	16.416	0.0312	1.0233	11.3628	0.014 244
Mn fcc	9.241	0.0289	0.5344	7.1614	0.015 949
Fe bcc	19.539	0.0333	1.3017	6.9299	0.007 299
Fe fcc	8.743	0.0309	0.5405	5.2622	0.012 386
Co bcc	19.809	0.0342	1.3534	4.8809	0.005 071
Co fcc	13.566	0.0336	0.9130	4.6340	0.007 030
Ni bcc	12.900	0.0339	0.8749	2.7626	0.004 407
Ni fcc	31.209	0.0344	2.1449	3.6851	0.002 430
Cu bcc	2.182	0.0201	0.0876	0.6868	0.006 478
Cu fcc	1.853	0.0211	0.0784	0.4574	0.005 079

According to the Vosko-Perdew theory[7] the exchange-enhanced susceptibility

$$X = N(E_F)/[1 - N(E_F)I_F] \ , \tag{3}$$

where the "exchange" integral is given by

$$I_F = \int dr\, \gamma^2(r)|K(r)| \tag{4}$$

with

$$\gamma = \frac{1}{N(E_F)} \sum_{\ell} N_\ell(E_F) R_\ell^2(E_F) \ , \tag{5}$$

where $R_\ell(E_F)$ is the radical wave function and $K(r)$ is a complicated function of the exchange-correlation potential,[7] which in turn depend on the charge density of the solid.[11] Negative values of X indicate ferromagnetic instability, so any element for which $N(E_F)I_F \geq 1$ (the so-called Stoner criterion) should be ferromagnetic.

For each element, the calculations were performed for lattice constants close to the computed equilibrium (the differences from the computed equilibrium were within 1%). Using our present and previous[1] self-consistent potentials, we performed a final APW calculation in order to find the band structure $E(\mathbf{k})$, which was used to compute the DOS by the tetrahedron method.[20] In the calculations of the DOS, we used 45 and 55 **k** points in the irreducible Brillouin zone (IBZ) for the hcp and bcc structures, respectively. While for the fcc structure, we found the $E(\mathbf{k})$ in 33 **k** points in the IBZ, which were then interpolated[21] to a 505 k-point mesh before the tetrahedron method was used; therefore, we expect more accurate results for the fcc structures.

B. Results

Our results are tabulated in Tables II, III, and IV for 3*d*, 4*d*, and 5*d* elements, respectively. The results are in good agreement (especially for the 4*d* metals) with previous calculations of the electron-phonon interactions for 3*d* and 4*d* elements in the fcc or bcc structures.[22] Some small discrepancies can be attributed to differences in the lattice constants.[23]

Figure 1 shows the $N(E_F)$ as a function of valence electrons Z for the 5*d* elements in bcc, fcc, and hcp structures. The trends for fcc and bcc structures also were presented in our previous paper (see Figs. 1 and 2 in Ref. 1). $N(E_F)$ for fcc structures is fairly constant across each

TABLE III. Electron-phonon interaction and Stoner criterion parameters for 4*d* metals.

System	$N(E_F)$ (Ry^{-1}/atom/spin)	I_F (Ry)	$I_F N(E_F)$	η (eV/Å^2)	$\langle I^2 \rangle$ (Ry/a.u.)^2
Sr bcc	4.852	0.0171	0.1658	0.2203	0.000 934
Sr fcc	0.001	0.0018	0.0000	0.0001	0.001 027
Y bcc	15.360	0.0163	0.5002	3.3444	0.004 481
Y fcc	10.076	0.0183	0.3695	2.5046	0.005 116
Y hcp	14.733	0.0180	0.5261	3.1834	0.004 485
Zr bcc	10.150	0.0159	0.3227	5.6925	0.011 542
Zr fcc	10.567	0.0181	0.3836	5.7588	0.011 216
Zr hcp	4.455	0.0176	0.1568	2.3229	0.010 731
Nb bcc	11.774	0.0166	0.3917	9.5701	0.016 728
Nb fcc	10.335	0.0188	0.3897	7.0135	0.013 966
Mo bcc	3.490	0.0184	0.1286	5.4504	0.032 140
Mo fcc	8.245	0.0181	0.2986	7.2099	0.017 996
Tc bcc	11.049	0.0214	0.4731	12.0774	0.022 495
Tc fcc	6.745	0.0203	0.2741	7.8937	0.024 087
Tc hcp	6.243	0.0192	0.2396	6.9220	0.022 816
Ru bcc	12.476	0.0229	0.5723	8.2450	0.013 601
Ru fcc	5.822	0.0206	0.2400	6.0977	0.021 553
Ru hcp	5.641	0.0220	0.2486	7.1509	0.026 089
Rh bcc	12.311	0.0232	0.5714	5.0356	0.008 418
Rh fcc	9.069	0.0227	0.4122	5.6991	0.012 933
Pd bcc	8.725	0.0229	0.4002	2.7157	0.006 406
Pd fcc	18.494	0.0230	0.8492	3.6649	0.004 078
Ag bcc	2.029	0.0152	0.0615	0.3571	0.003 622
Ag fcc	1.800	0.0165	0.0594	0.2913	0.003 331

row but abruptly increase to a maximum for $Z=10$ (Ni,Pd,Pt) column; there are wider variations for $N(E_F)$ of bcc structures with a pronounced minimum at $Z=6$ (Cr,Mo,W) and two well-defined maxima at $Z=3$ (Sc,Y,La) and $Z=9$ (Co,Rh,Ir). The present results for $N(E_F)$ of hcp structures show an oscillatory behavior with three maxima at $Z=3$ (Sc,Y,La), 6 (Cr,Mo,W), and 10 (Ni,Pd,Pt). We have hcp results for a complete row only for the 5*d* elements, but, as for the bcc and fcc structures (see Tables II–IV and Figs. 1 and 2 in Ref. 1), we expect the same behavior for all the rows.

The exchange integral I_F for the 5*d* elements is found in Table IV. The I_F is almost identical; for fcc and hcp structures it has a minimum at $Z=3$ La. It then increases constantly until reaching maximum values at $Z=9,10$ (Ir,Pt), then drops sharply. For bcc structures, I_F has a maximum at $Z=9$ (Ir) and is significantly smaller than I_F for fcc and hcp structures at $Z=10$ (Pt). Also, the I_F for bcc structures does not exhibit the sharp minimum at $Z=3$ (La), which appears in fcc and hcp structures. The product $N(E_F)\times I_F$ (Fig. 2 and Table IV) follows closely the variation of the $N(E_F)$; the maxima and minima of that product appear at exactly the same Z as in $N(E_F)$ for all the structures (compare Figs. 1 and 2). The I_F does not vary too much along each row; in particular for the 5*d* and for all the structures it has a 44% variation from its average value. However, this variation is crucial in determining whether $N(E_F)\times I_F$ satisfies the Stoner criterion. Recently, Bakonyi, Ebert, and Liechtenstein[24] calculated the exchange integral I_F and the Stoner enhancement factor $S(=1/[1-N(E_F)I_F])$ for the hcp, bcc, and fcc structures of the element in the fourth column of the Periodic Table (Ti,Zr,Hf). The I_F for Ti is almost identical with

TABLE IV. Electron-phonon interaction and Stoner criterion parameters for 5*d* metals.

System	$N(E_F)$ (Ry^{-1}/atom/spin)	I_F (Ry)	$I_F N(E_F)$	η (eV/Å^2)	$\langle I^2\rangle$ (Ry/a.u.)^2
Ba bcc	7.470	0.0149	0.2219	0.5269	0.001 451
Ba fcc	10.625	0.0169	0.3590	0.6199	0.001 201
Ba hcp	13.536	0.0173	0.2346	0.4402	0.001 339
La bcc	36.638	0.0143	1.0455	5.6662	0.003 183
La fcc	14.479	0.0135	0.3918	3.0098	0.004 278
La hcp	18.467	0.0142	0.5233	2.9027	0.003 235
Hf bcc	11.180	0.0155	0.3466	5.4119	0.009 962
Hf fcc	10.966	0.0177	0.3885	6.8864	0.012 924
Hf hcp	5.280	0.0174	0.1832	2.8029	0.010 925
Ta bcc	10.366	0.0162	0.3351	9.8476	0.019 552
Ta fcc	7.508	0.0177	0.2653	6.4856	0.017 777
Ta hcp	10.341	0.0173	0.3577	7.8481	0.015 619
W bcc	2.805	0.0181	0.1018	4.5406	0.033 309
W fcc	8.586	0.0185	0.3172	7.2500	0.017 377
W hcp	14.151	0.0176	0.4972	14.7475	0.021 448
Re bcc	8.541	0.0195	0.3334	14.1792	0.034 166
Re fcc	5.460	0.0191	0.2083	7.7874	0.029 351
Re hcp	4.107	0.0180	0.1475	5.8268	0.029 198
Os bcc	9.037	0.0207	0.3740	8.5526	0.019 476
Os fcc	4.500	0.0192	0.1727	6.6792	0.030 548
Os hcp	4.168	0.0199	0.1657	6.1402	0.030 319
Ir bcc	23.474	0.0215	1.0078	8.1585	0.007 153
Ir fcc	6.884	0.0211	0.2902	6.7453	0.020 165
Ir hcp	8.682	0.0217	0.3766	8.5160	0.020 185
Pt bcc	6.876	0.0192	0.2646	4.5660	0.013 667
Pt fcc	13.587	0.0217	0.5896	4.8350	0.007 324
Pt hcp	14.725	0.0220	0.6486	6.5233	0.009 117
Au bcc	1.968	0.0138	0.0543	0.7057	0.007 380
Au fcc	1.716	0.0145	0.0497	0.4900	0.005 876
Au hcp	2.082	0.0145	0.0602	0.8129	0.008 033

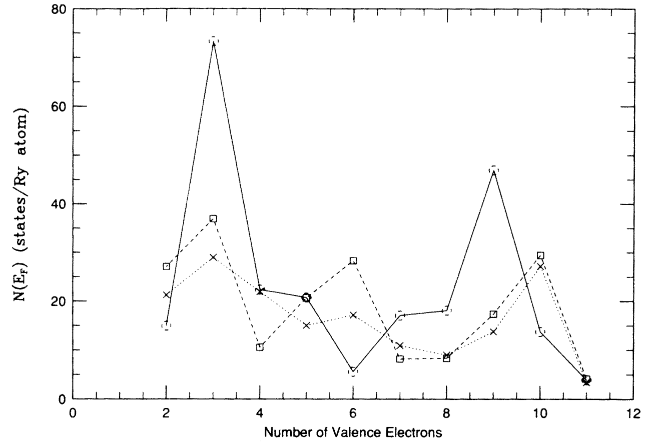

FIG. 1. The density of states $N(E_F)$ at the Fermi energy E_F vs the number of valence electrons for $5d$ metals in bcc (circles), fcc (crosses), and hcp (squares) structures.

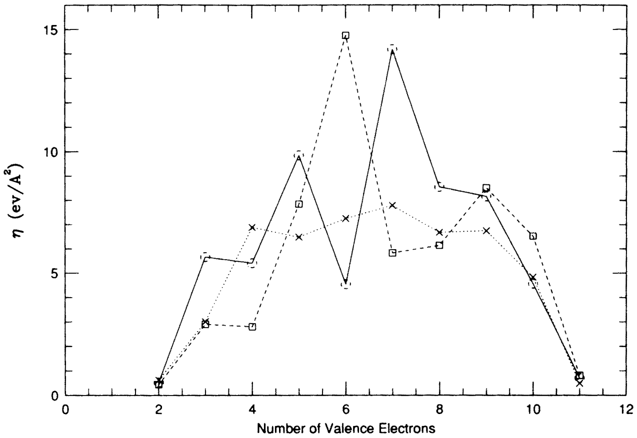

FIG. 3. η vs the number of valence electrons for $5d$ metals in bcc (circles), fcc (crosses), and hcp (squares) structures.

the present results while for the other elements the agreement is very good. The S for hcp structures are almost the same as present results, but there are some differences in the values of S for fcc and bcc structures, which come from the differences of $N(E_F)$. Bakonyi, Ebert, and Liechtenstein found that $N(E_F)$ for the bcc structure are slightly higher than $N(E_F)$ for fcc, while our results show exactly the opposite feature.

The square of the electron ion matrix element averaged over the Fermi surface $\langle I^2 \rangle$ (see Table IV) has the same trend for both fcc and hcp structures; it increases as the Z increases until it reaches its maximum value at $Z=7,8$ (Re,Os); then it decreases as the Z increases. For $Z \leq 5$, $\langle I^2 \rangle$ of bcc structures is almost the same with $\langle I^2 \rangle$ of both fcc and hcp structures, but for higher Z there are considerable differences. The maximum of $\langle I^2 \rangle$ for bcc structures appears at $Z=6,7$ (W,Re), while its bcc values for $Z=8,9$ (Os,Ir) are much smaller than the $\langle I^2 \rangle$ for fcc and hcp structures. The McMillan-Hopfield parameter η (see Fig. 3 and Table IV) for fcc structures has an almost parabolic form across the d series with its maximum value at $Z=7$ (Re). For bcc structures, η has one maximum at $Z=5$ (Ta) and another even higher maximum at $Z=7$ (Re). On the other hand, for hcp structures, η has a sharp maximum at $Z=6$ (W) and a smaller one at $Z=9$ (Ir). Notice also that the maximum values of η (~ 14.5 eV/Å^2) for W hcp and Re bcc are more than twice higher than the corresponding values of those elements at their equilibrium structures (W bcc and Re hcp). This suggests possible higher superconducting temperatures for the metastable structures.

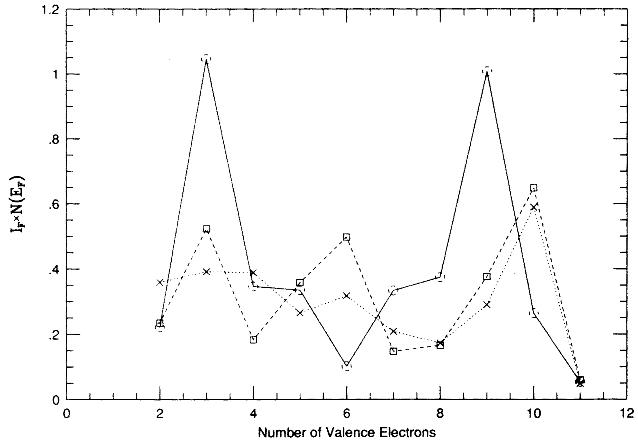

FIG. 2. $I_F \times N(E_F)$ vs the number of valence electrons for $5d$ metals in bcc (circles), fcc (crosses), and hcp (squares) structures.

Comparing the values of the various parameters among the three different series (see Tables II–IV), we find that for the same structure η is almost the same for all the elements at the same column of the Periodic Table. The same behavior exists for the Stoner criterion, $I_F \times N(E_F)$, between the $4d$ and $5d$ elements. In contrast, the value of $I_F N(E_F)$ for the $3d$ element is considerably higher although the general trends are the same for all the series. This is basically a consequence of the high values of I_F in the $3d$ series; the I_F for $3d$ elements is about 50% higher than the corresponding elements at $4d$ and $5d$ series (Tables II–IV). This is consistent with the occurrence of magnetism in the $3d$ elements. From Tables II–IV, we note that the following materials bcc Mn, bcc Fe, bcc Co, fcc Ni, bcc La, and bcc Ir satisfy the Stoner criterion, while fcc Co, bcc Ni, fcc Pd, and hcp Pt have $I_F \times N(E_F)$ very close to the critical value of 1.0. Note that $I_F N(E_F)$ is actually a lower bound to the exact result.[7]

Finally, to study the volume dependence of the above parameters that control superconductivity and magnetism, we present in Table V the values of these parameters for fcc Pt at five different lattice constants, a. I_F is almost constant over a wide region of a. $N(E_F)$ and $I_F N(E_F)$ increases as the lattice constant increases. In constant, $\langle I^2 \rangle$ decreases rapidly as a increases; the $\langle I^2 \rangle$ for a = 7.2 a.u. is almost two times greater than the $\langle I^2 \rangle$ for $a=7.6$ a.u. Finally, η exhibits the same behavior as $\langle I^2 \rangle$ but the changes of η with a are smaller than those of $\langle I^2 \rangle$, since η is also dependent on $N(E_F)$ [Eq. (1)].

TABLE V. Lattice constant variation of the density of states electron-phonon interaction and Stoner parameters for Pt.

Lat. const.	E_F (Ry)	$N(E_F)$ (States/Ry)	I_F (Ry)	$I_F N(E_F)$	η (eV/Å^2)	$\langle I^2 \rangle$ (Ry/a.u.)^2
7.2	0.7544	11.690	0.021 84	0.5105	5.9884	0.010 543
7.3	0.6951	12.914	0.021 75	0.5617	5.4323	0.008 657
7.4	0.6438	13.587	0.021 70	0.5896	4.8350	0.007 324
7.5	0.5938	14.689	0.021 60	0.6347	4.4379	0.006 218
7.6	0.5470	15.961	0.021 50	0.6862	4.0854	0.005 268

IV. CONCLUSIONS

We calculated the total energies of all the metals crystallizing in hcp structures and all the 5*d* metals in the hcp structure. Equilibrium lattice constants and bulk moduli in the local-density approximation have the usual small discrepancies from experiment. We also studied the electron-phonon interaction and the magnetic properties of transition metals. The metals with valence electrons $Z=5$ (V,Nb,Ta) at their equilibrium bcc structures, $Z=6$ (Cr,Mo,W) at their metastable hcp structures, and $Z=7$ (Mn,Tc,Re) at their metastable bcc structures have high electron-phonon parameter, η. The Stoner criterion $[I_F \times N(E_F) \geq 1]$ is fulfilled for all the elements at the end of the 3*d* series in accordance with the occurrence of ferromagnetism for those metals. For elements in the 4*d* and 5*d* series, bcc La and bcc Ir fulfill the Stoner criterion, while fcc Pd and hcp Pt are very close to fulfilling it. Note that from those metals only fcc Pd is in its equilibrium structure.

ACKNOWLEDGMENTS

Ames Laboratory is operated by the U.S. Department of Energy by Iowa State University under Contract No. W-7405-Eng-82.

---

[1] M. Sigalas, D. A. Papaconstantopoulos, and N. C. Bacalis, Phys. Rev. B **45**, 5777 (1992).

[2] M. Sigalas, N. C. Bacalis, D. A. Papaconstantopoulos, M. J. Mehl, and A. C. Switendick, Phys. Rev. B **42**, 11 637 (1990).

[3] L. Cortella, B. Vinet, P. J. Desré, A. Pasturel, A. T. Paxton, and M. van Schilfgaarde, Phys. Rev. Lett. **70**, 1469 (1993).

[4] M. M. Sigalas and D. A. Papaconstantopoulos, Phys. Rev. B **49**, 1574 (1994); M. M. Sigalas and D. A. Papaconstantopoulos, in *Materials Theory and Modelling,* edited by J. Broughton, P. Bristowe, and J. Newsam, MRS Symposia Proceedings No. 291 (Materials Research Society, Pittsburgh, 1993), p. 27.

[5] H. B. Shore and J. H. Rose, Phys. Rev. Lett. **66**, 2519 (1991); (unpublished).

[6] G. D. Gaspari and B. L. Gyorffy, Phys. Rev. Lett. **28**, 801 (1972).

[7] S. H. Vosko and J. P. Perdew, Can. J. Phys. **53**, 1385 (1975); D. Gunnarsson, J. Phys. F 6, 587 (1976); J. F. Janak, Phys. Rev. B **16**, 255 (1977).

[8] J. F. Janak, Phys. Rev. B **9**, 3985 (1974).

[9] L. F. Mattheiss, J. H. Wood, and A. C. Switendick, Methods Comput. Phys. **8**, 63 (1968).

[10] D. D. Koelling and B. N. Harmon, J. Phys. C **10**, 3107 (1977).

[11] L. Hedin and B. I. Lundqvist, J. Phys. C **4**, 2064 (1971).

[12] C. Kittell, *Introduction to Solid State Physics* (Wiley, New York, 1986).

[13] A. T. Paxton, M. Methfessel, and H. M. Polatoglou, Phys. Rev. B **41**, 8127 (1990).

[14] J. P. Perdew, J. A. Chevary, S. H. Vosko, K. A. Jackson, M. R. Pederson, D. J. Singh, and C. Fiolhais, Phys. Rev. B **46**, 6671 (1992).

[15] J. P. Perdew, Phys. Rev. B **34**, 7406 (1986); D. C. Langreth and M. J. Mehl, Phys. Rev. Lett. **47**, 446 (1981).

[16] D. J. Singh (private communication).

[17] G. W. Fernando, R. E. Watson, M. Weinert, Y. J. Wang, and J. W. Davenport, Phys. Rev. B **41**, 11 813 (1990).

[18] H. L. Skriver, Phys. Rev. B **31**, 1909 (1984).

[19] D. G. Pettifor, J. Phys. C **3**, 367 (1970).

[20] G. Lehmann and M. Taut, Phys. Status Solidi **54**, 469 (1972).

[21] L. L. Boyer, Phys. Rev. B **19**, 2824 (1979).

[22] D. A. Papaconstantopoulos, L. L. Boyer, B. M. Klein, A. R. Williams, V. L. Moruzzi, and J. F. Janak, Phys. Rev. B **15**, 4221 (1977).

[23] C.-G. Jiang, G. Fletcher, J. L. Fry, and D. A. Papaconstantopoulos, Phys. Rev. B **44**, 2268 (1991).

[24] I. Bakonyi, H. Ebert, and A. I. Liechtenstein, Phys. Rev. B **48**, 7841 (1993).