Screening Dependence Study of Superconducting State Parameters of 4*d*- and 5*d*-Transition Metals Based Binary Alloys

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Screening dependence study of the superconductivity in 4*d*- and 5*d*-transition metals based binary alloys was performed using the model pseudopotential approach, which was found quite successful in explaining superconductivity in metals, alloys, and metallic glasses. In the present work the superconducting state parameters viz. electron–phonon coupling strength λ, the Coulomb pseudopotential μ^*, transition temperature T_C, isotope effect exponent α and effective interaction strength N_0V of some transition metals based binary alloys of 4*d*- and 5*d*-transition metals groups were determined in the BCS–Eliashberg–McMillan framework. A considerable influence of various exchange and correlation functions on λ and μ^* is found from the present study. The present results of the superconducting state parameters are found in qualitative agreement with the available experimental figures wherever exist.

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1. Introduction

Superconductivity phenomenon has been beguiling and bedeviling physicists for a century while numerous other quaint and curious collective phenomena have been discovered and analyzed, yet it maintains its mystery in spite of the enormous amount that has been learned and the vast competition for the physical scientist's attention and devotion. The simple problem of determining the superconducting transition temperature T_C of a superconductor has two separate parts viz. first one of understanding the material properties such as electron–phonon coupling strength λ, the Coulomb pseudopotential μ^* and the phonon spectrum which is usually oversimplified by some frequency ω and second one of calculating transition temperature T_C which depends on such properties. Such paper is to provide links to the first part. With the improved information of the phonon spectrum and electron–ion coupling, more accurate calculations of these parameters have been made, where one uses the theory of superconductivity, with its sophisticated Green's-function formalism taking into account the retarded electron–phonon interaction and including the important energy renormalization effects due to many-body interactions [1–23]. The electron–phonon (EP) interaction is an important process in solids and the most dramatic manifestation of this interaction is superconductivity in metals, where all of the properties are drastically modified with respect to the normal (non-superconducting) state [24].

In earlier communications [3–17], we have intended the superconducting state parameters (SSP) electron–phonon coupling strength λ and Coulomb pseudopotential μ^*, and hence the transition temperature T_C, the isotope effect exponent α and effective interaction strength N_0V using various forms of screening with model potential formalism for metals, alloys and metallic glasses. Earlier, we have reported screening dependence study of superconducting state parameters of some 3*d*-transition metals based binary alloys using model potential approach [17]. But, in the present paper, we only focus our attention to study the screening dependence on the superconducting properties of some 4*d*- and 5*d*-transition metals based binary alloys. In all these former studies, we made the drastic approximation of replacing the mean square phonon frequency $\langle\omega^2\rangle$ by θ_{D}, the Debye temperature, which incidentally could not provide a sufficiently reliable assessment of the phonon spectrum for a weak-coupling superconductor. Moreover, a systematic search for an accurate and accessible characteristic temperature has not yet been made but would be of considerable value. Therefore, we use $\langle\omega^2\rangle$ to estimate the parameters λ and μ^* as suggested by Allen and Cohen [22] and adopt the most reliable values of band structure mass m_b [23]. Such considerations are liable to reproduce satisfactorily the values of SSP for 4*d*- and 5*d*-transition metals based binary alloys. Bose [24] has reported pressure dependence electron–phonon coupling and spin fluctuations in 3*d*- and 4*d*-transition metals using the linear response method and the linear muffin-tin orbitals' basis. He pointed out that spin fluctuations play an important role in the validity of the Matthias rule [25, 26] that in metallic systems the optimum conditions for (electron–phonon) superconductivity occur for 5 and 7 valence electrons/atom. Superconductivity in transition metals has been studied by Peretti [27] using Garland's model. He noted that the *s*–*d* interaction leads to superconductivity. Pettifor [28] reported variation of the electronic contribution (η) to the electron–phonon mass enhancement factor of electron–phonon coupling strength (λ) which is studied across the 4*d*-transition metal series within the Gaspari-Gyorffy rigid-muffin-tin (RMT) approximation. Ratti et al. [29] reported the volume dependence of the width of the *d*-resonance in some transition metals using the Matthias [25, 26] prescription for the crystalline

electron–ion potential.

The application of pseudopotential to binary alloys involves the assumption of pseudoions with average properties, which are assumed to replace three types of ions in the binary systems, and a gas of free electrons is supposed to permeate through them. The electron–pseudoion is accounted for by the pseudopotential and the electron–electron interaction is involved through a dielectric screening function. For successful prediction of the superconducting properties of the alloying systems, the proper selection of the pseudopotential and screening function is very essential [3–19].

In the present article, well recognized model potential of Patel and co-workers [30, 31] is applied in the present study of the SSP viz. electron–phonon coupling strength λ, the Coulomb pseudopotential μ^*, transition temperature T_C, isotope effect exponent α and effective interaction strength N_0V of transition metals based binary alloys. To see the influence of various exchange and correlation functions on the aforesaid properties, we have used five different types of local field correction functions suggested by Hartree (H) [32], Taylor (T) [33], Ichimaru–Utsumi (IU) [34], Farid et al. (F) [35] and Sarkar et al. (S) [36]. We have employed here pseudo-alloy-atom (PAA) model used to explain electron–ion interaction for binary superconductors. Such model is a more meaningful method to explain such kind of interactions in binary systems [3–17].

2. Computational methodology

In the present investigation for binary mixtures, the electron–phonon coupling strength λ is computed using the relation [3–19]:

$$\lambda = \frac{m_b \Omega_0}{4\pi^2 k_f m \langle\omega^2\rangle} \int_0^{2k_f} q^3 \left|W\left(q\right)\right|^2 \mathrm{d}q. \tag{1}$$

Here m_b is the band mass, M — the ionic mass, Ω_0 — the atomic volume, k_f — the Fermi wave vector and $W\left(q\right)$ — the screened pseudopotential. The mathematical expression of $W\left(q\right)$ is narrated in their respective paper [30, 31]. The effective averaged square phonon frequency $\left\langle\omega^2\right\rangle$ is calculated using the relation given by Butler [37] viz. $\left\langle\omega^2\right\rangle^{1/2} = 0.69\theta_{\mathrm{D}}$, where θ_{D} is the Debye temperature of the transition metals based binary alloys.

Using $X = q/2k_f$ and $\Omega_0 = 3\pi^2 Z/k_f^3$, we get Eq. (2) in the following form:

$$\lambda = \frac{12 m_b Z}{m\langle\omega^2\rangle} \int_0^1 X^3 \left|W\left(X\right)\right|^2 \mathrm{d}X. \tag{2}$$

Here, Z is the valence of the transition metals based binary alloys. The Coulomb pseudopotential μ^* is given by [3–19]:

$$\mu^* = \frac{\frac{m_b}{\pi k_f}\int_0^1 \frac{\mathrm{d}X}{\varepsilon(X)}}{1 + \frac{m_b}{\pi k_f}\ln\left(\frac{E_f}{10\theta_{\mathrm{D}}}\right)\int_0^1 \frac{\mathrm{d}X}{\varepsilon(X)}}, \tag{3}$$

where E_f is the Fermi energy, m_b — the band mass of the electron and $\varepsilon\left(X\right)$ — the modified Hartree dielectric function, which is written as [32]:

$$\varepsilon\left(X\right) = 1 + \left(\varepsilon_{\mathrm{H}}\left(X\right) - 1\right)\left(1 - f\left(X\right)\right). \tag{4}$$

$\varepsilon_{\mathrm{H}}\left(X\right)$ is the static Hartree dielectric function [32] and $f\left(X\right)$ — the local field correction function. In the present investigation, the local field correction functions due to H, T, IU, F, and S are incorporated to see the influence of exchange and correlation effects. The details of all the local field corrections are discussed in their respective papers [32–36]. After estimating λ and μ^*, the superconducting transition temperature T_C and isotope effect exponent α are investigated from the McMillan formula [3–21]:

$$T_C = \frac{\theta_{\mathrm{D}}}{1.45}\exp\left(\frac{-1.04\left(1+\lambda\right)}{\lambda - \mu^*\left(1+0.62\lambda\right)}\right), \tag{5}$$

$$\alpha = \frac{1}{2}\left[1 - \left(\mu^* \ln\frac{\theta_{\mathrm{D}}}{1.45T_C}\right)^2 \frac{1+0.62\lambda}{1.04\left(1+\lambda\right)}\right]. \tag{6}$$

The expression for the effective interaction strength N_0V is studied using [3–19]:

$$N_0V = \frac{\lambda - \mu^*}{1 + \frac{10}{11}\lambda}. \tag{7}$$

3. Results and discussion

The constants and parameters used in the present study are tabulated in Tables I and II. To determine the input parameters and various constants, we use PAA model [3–17] in the present computation for transition metals based binary alloys ($A_{1-x}B_x$). Here, x is concentration factor of the second metallic component of the alloys.

TABLE I

Input parameters and other constants of 4*d*-transition metals based binary alloys.

Alloy	Z	r_C [a.u.]	Ω_0 [a.u.^{3}]	M [amu]	θ_{D} [K]
$Zr_{0.50}Nb_{0.50}$	4.50	0.7085	131.98	91.62	238.00
$Zr_{0.25}Nb_{0.75}$	4.75	0.7008	119.60	91.81	246.00
$Nb_{0.85}Mo_{0.15}$	5.15	0.7894	106.91	92.6	265.00
$Nb_{0.60}Mo_{0.40}$	5.40	0.7644	106.39	93.58	370.00
$Nb_{0.40}Mo_{0.60}$	5.60	0.7678	105.98	94.37	429.00
$Nb_{0.30}Mo_{0.70}$	5.70	0.7835	105.78	94.76	442.00
$Nb_{0.20}Mo_{0.80}$	5.80	0.7169	105.57	95.15	461.00
$Nb_{0.10}Mo_{0.90}$	5.90	0.6585	105.37	95.55	487.00
$Mo_{0.95}Re_{0.05}$	6.05	0.6369	104.86	100.45	450.00
$Mo_{0.90}Re_{0.10}$	6.10	0.6038	104.56	104.97	440.00
$Mo_{0.80}Re_{0.20}$	6.20	0.5292	103.97	113.99	420.00
$Mo_{0.70}Re_{0.30}$	6.30	0.5189	103.37	123.02	395.00
$Mo_{0.60}Re_{0.40}$	6.40	0.5574	102.77	132.05	340.00
$Mo_{0.50}Re_{0.50}$	6.50	0.5845	102.18	141.08	320.00
$Mo_{0.50}Tc_{0.50}$	6.50	0.7091	100.76	97.43	300.00
$Zr_{0.97}Rh_{0.03}$	3.97	0.7509	154.78	91.54	244.00
$Zr_{0.96}Rh_{0.04}$	3.96	0.7769	154.13	91.65	226.00
$Zr_{0.95}Rh_{0.05}$	3.95	0.7930	153.47	91.75	210.00
$Zr_{0.94}Rh_{0.06}$	3.94	0.8079	152.82	91.86	196.00
$Zr_{0.93}Rh_{0.07}$	3.93	0.8135	152.16	91.97	192.00

TABLE II

Input parameters and other constants of 5*d*-transition metals based binary alloys.

Alloy	Z	r_C [a.u.]	Ω_0 [a.u.^{3}]	M [amu]	θ_D [K]
$Hf_{0.30}Ta_{0.70}$	4.70	0.6209	130.61	180.21	209
$Re_{0.30}Os_{0.70}$	4.90	0.4661	95.81	181.41	382
$Ta_{0.84}W_{0.16}$	5.16	0.6080	121.43	182.11	265
$Ta_{0.60}W_{0.40}$	5.40	0.6241	121.07	182.69	291
$Ta_{0.40}W_{0.60}$	5.60	0.6375	120.76	183.27	317
$Ta_{0.20}W_{0.80}$	5.80	0.6444	120.46	183.56	354
$Ta_{0.10}W_{0.90}$	5.90	0.6929	120.31	183.97	368
$W_{0.95}Re_{0.05}$	6.05	0.6366	119.11	184.03	380
$W_{0.925}Re_{0.075}$	6.08	0.5877	118.59	184.09	378
$W_{0.90}Re_{0.10}$	6.10	0.5858	118.06	184.2	375
$Re_{0.70}Os_{0.30}$	6.10	0.6046	97.74	184.32	351
$W_{0.85}Re_{0.15}$	6.15	0.5447	117.01	184.44	365
$W_{0.80}Re_{0.20}$	6.20	0.5350	115.97	185.93	359
$W_{0.75}Re_{0.25}$	6.25	0.5227	114.92	187.41	351
$W_{0.88}Re_{0.12}$	6.88	0.5616	101.71	189.00	332

Tables III and IV show presently calculated values of the SSP viz. electron–phonon coupling strength λ, the Coulomb pseudopotential μ^*, transition temperature T_C, isotope effect exponent α and effective interaction strength N_0V at various concentrations for 4*d*- and 5*d*-transition metals based binary alloys with available experimental [21] and theoretical [3–5] findings.

From Tables II–III it can be noted that the λ goes on decreasing from the values of 1.5560→0.4639 as the concentration x of Mo is increased from 0.15→0.90, while for concentration x of Nb, Re and Rh increases, while the λ goes on increasing in the range of 0.7904→1.3138, 0.5523→1.2582, and 0.4502→1.0285, respectively. The overall percentile difference found between computed data of electron–phonon coupling strength λ for 4*d*-transition metals based binary alloys with experimental one is found in the range of 0.11%–0.93%. From Table III it results that the λ goes on decreasing from the values of 0.9613→0.5016 and 1.0218→0.3973 as the concentration x of W and Os is increased, respectively, while λ goes on increasing from 0.5047→1.4379 for concentration x of Re increases from 0.05→0.50. Similarly, the overall percentile difference found between computed data of electron–phonon coupling strength λ for 5*d*-transition metals based binary alloys with experimental data lies in the range of 0.25%–0.82%. The increase or decrease nature in λ with concentration x of second metallic elements shows a continuing transition from weak to intermediate coupling behaviour of electrons and phonons, which may be recognized to an increase of the hybridization of *sp*–*d* electrons. It is attributed to the increasing role of ionic vibrations in the 4*d*- or 5*d*-transtion metals rich region. Also, the present results are found in qualitative agreement with the available experimental [21] and theoretical [3–5] data.

Superconducting state parameters of the 4*d*-transition metals based binary alloys. T_C [K]. TABLE III

Alloys	SSP	Present result					Exp.	Theor. [3, 4]
		H	T	IU	F	S	[21]	
$Zr_{0.50}Nb_{0.50}$	λ	0.7903	1.0502	1.0946	1.0969	0.9432	0.88	0.8547, 1.1553, 1.2078, 1.2123, 1.0206
	μ^*	0.1908	0.1998	0.2010	0.2012	0.1957	–	0.1195, 0.1282, 0.1293, 0.1296, 0.1242
	T_C	4.1404	8.5005	9.2396	9.2696	6.7392	9.3	9.3015, 14.9414, 15.8244, 15.8917, 12.5716
	α	0.3026	0.3644	0.3710	0.3711	0.3468	–	0.4534, 0.4639, 0.4651, 0.4652, 0.4605
	N_0V	0.3488	0.4350	0.4478	0.4484	0.4024	–	0.4138, 0.5010, 0.5140, 0.5151, 0.4650
$Zr_{0.25}Nb_{0.75}$	λ	0.9587	1.2605	1.3110	1.3138	1.1303	0.93	0.8995, 1.1955, 1.2460, 1.2498, 1.0604
	μ^*	0.1898	0.1982	0.1993	0.1995	0.1943	–	0.1170, 0.1252, 0.1263, 0.1265, 0.1212
	T_C	7.6019	12.7145	13.5042	13.5370	10.6361	10.8	10.8032, 16.4101, 17.2635, 17.3179, 14.0242
	α	0.3639	0.4000	0.4040	0.4040	0.3889	–	0.4591, 0.4674, 0.4684, 0.4684, 0.4647
	N_0V	0.4108	0.4950	0.5072	0.5077	0.4616	–	0.4305, 0.5129, 0.5250, 0.5259, 0.4782
$Nb_{0.85}Mo_{0.15}$	λ	1.1533	1.4968	1.5529	1.5560	1.3383	0.70	0.6643, 0.8474, 0.8748, 0.8760, 0.7698
	μ^*	0.1897	0.1974	0.1984	0.1986	0.1934	–	0.1143, 0.1220, 0.1230, 0.1232, 0.1179
	T_C	12.2182	17.8423	18.6536	18.6882	15.4496	5.85	5.8528, 10.0027, 10.6126, 10.6288, 8.3132
	α	0.3990	0.4216	0.4241	0.4241	0.4140	–	0.4369, 0.4501, 0.4515, 0.4514, 0.4467
	N_0V	0.4703	0.5504	0.5616	0.5621	0.5164	–	0.3429, 0.4098, 0.4188, 0.4191, 0.3835
$Nb_{0.60}Mo_{0.40}$	λ	0.6587	0.8520	0.8833	0.8850	0.7610	0.41	0.3834, 0.4887, 0.5046, 0.5053, 0.4428
	μ^*	0.2017	0.2102	0.2113	0.2115	0.2057	–	0.1178, 0.1260, 0.1271, 0.1273, 0.1216
	T_C	2.5510	6.7694	7.5441	7.5768	4.6898	0.60	0.6006, 2.1685, 2.4906, 2.4972, 1.3945
	α	0.1475	0.2689	0.2812	0.2813	0.2283	–	0.2812, 0.3480, 0.3547, 0.3544, 0.3295
	N_0V	0.2858	0.3616	0.3727	0.3732	0.3282	–	0.1970, 0.2511, 0.2588, 0.2590, 0.2291
$Nb_{0.40}Mo_{0.60}$	λ	0.5319	0.6863	0.7111	0.7125	0.6125	0.31	0.2961, 0.3755, 0.3872, 0.3877, 0.3407
	μ^*	0.2072	0.2160	0.2172	0.2174	0.2112	–	0.1190, 0.1273, 0.1284, 0.1286, 0.1228
	T_C	0.5915	2.8671	3.3889	3.4108	1.5931	0.05	0.0501, 0.4245, 0.5277, 0.5297, 0.2075
	α	-0.1923	0.0920	0.1184	0.1189	-0.0012	–	0.0311, 0.2005, 0.2160, 0.2155, 0.1547
	N_0V	0.2188	0.2895	0.2999	0.3004	0.2577	–	0.1395, 0.1850, 0.1914, 0.1916, 0.1664

TABLE III (cont.)

Alloys	SSP	Present result					Exp.	Theor. [3, 4]
		H	T	IU	F	S	[21]	
$Nb_{0.30}Mo_{0.70}$	λ	0.5215	0.6719	0.6961	0.6975	0.5995	0.29	0.2737, 0.3455, 0.3557, 0.3562, 0.3140
	μ^*	0.2081	0.2170	0.2181	0.2183	0.2121	–	0.1190, 0.1273, 0.1284, 0.1286, 0.1227
	T_C	0.4908	2.5847	3.0784	3.0992	1.3875	0.016	0.0161, 0.1996, 0.2545, 0.2561, 0.0868
	α	-0.2495	0.0634	0.0922	0.0927	-0.0397	–	-0.1070, 0.1218, 0.1413, 0.1408, 0.0611
	N_0V	0.2125	0.2824	0.2927	0.2932	0.2507	–	0.1238, 0.1660, 0.1717, 0.1719, 0.1488
$Nb_{0.20}Mo_{0.80}$	λ	0.4986	0.6417	0.6646	0.6659	0.5723	0.33	0.3101, 0.3956, 0.4089, 0.4095, 0.3562
	μ^*	0.2096	0.2185	0.2196	0.2199	0.2136	–	0.1192, 0.1276, 0.1286, 0.1289, 0.1229
	T_C	0.3039	1.9801	2.4046	2.4224	0.9812	0.095	0.0953, 0.6922, 0.8567, 0.8601, 0.3393
	α	-0.3923	-0.0044	0.0303	0.0309	-0.1319	–	0.0907, 0.2377, 0.2522, 0.2518, 0.1939
	N_0V	0.1988	0.2672	0.2773	0.2778	0.2359	–	0.1489, 0.1972, 0.2043, 0.2045, 0.1762
$Nb_{0.10}Mo_{0.90}$	λ	0.4643	0.5968	0.6181	0.6193	0.5321	0.36	0.3444, 0.4439, 0.4599, 0.4609, 0.3945
	μ^*	0.2117	0.2207	0.2219	0.2221	0.2157	–	0.1196, 0.1280, 0.1291, 0.1293, 0.1233
	T_C	0.1189	1.1926	1.5047	1.5178	0.5061	0.30	0.3009, 1.5946, 1.9219, 1.9368, 0.8195
	α	-0.6968	-0.1395	-0.0918	-0.091	-0.3200	–	0.1943, 0.3009, 0.3120, 0.3120, 0.2641
	N_0V	0.1776	0.2438	0.2536	0.2541	0.2132	–	0.1712, 0.2251, 0.2333, 0.2337, 0.1996
$Mo_{0.95}Re_{0.05}$	λ	0.5523	0.7085	0.7335	0.7349	0.6313	0.45	0.4276, 0.5518, 0.5719, 0.5733, 0.4882
	μ^*	0.2077	0.2162	0.2173	0.2175	0.2114	–	0.1179, 0.1260, 0.1270, 0.1272, 0.1213
	T_C	0.8473	3.5435	4.1266	4.1514	2.0238	1.5	1.5015, 4.5753, 5.2008, 5.2352, 2.8568
	α	-0.1251	0.1210	0.1442	0.1446	0.0356	–	0.3318, 0.3826, 0.3882, 0.3883, 0.3638
	N_0V	0.2294	0.2994	0.3096	0.3101	0.2667	–	0.2230, 0.2836, 0.2927, 0.2932, 0.2541
$Mo_{0.90}Re_{0.10}$	λ	0.5658	0.7254	0.7508	0.7522	0.6461	0.51	0.4864, 0.6308, 0.6544, 0.6564, 0.5539
	μ^*	0.2065	0.2149	0.2160	0.2162	0.2102	–	0.1173, 0.1254, 0.1264, 0.1266, 0.1208
	T_C	1.0380	3.9675	4.5801	4.606	2.3347	2.9	2.9530, 7.3847, 8.2153, 8.2760, 4.8998
	α	-0.0704	0.1488	0.1697	0.1700	0.0718	–	0.3757, 0.4110, 0.4150, 0.4151, 0.3968
	N_0V	0.2372	0.3075	0.3178	0.3183	0.2746	–	0.2559, 0.3212, 0.3311, 0.3318, 0.2881
$Mo_{0.80}Re_{0.20}$	λ	0.5985	0.7662	0.7928	0.7943	0.6822	0.68	0.6492, 0.8500, 0.8828, 0.8868, 0.7344
	μ^*	0.2042	0.2123	0.2133	0.2135	0.2076	–	0.1162, 0.1241, 0.1251, 0.1253, 0.119
	T_C	1.5677	5.0221	5.6974	5.7265	3.1399	8.5	8.5066, 15.7302, 16.9035, 17.0362, 11.5863
	α	0.0316	0.2023	0.2189	0.2191	0.1408	–	0.4312, 0.4481, 0.4501, 0.4502, 0.4403
	N_0V	0.2553	0.3264	0.3367	0.3372	0.2928	–	0.3352, 0.4095, 0.4203, 0.4216, 0.3687
$Mo_{0.70}Re_{0.30}$	λ	0.6560	0.8388	0.8677	0.8693	0.7464	0.76	0.7210, 0.9432, 0.9795, 0.9840, 0.8134
	μ^*	0.2013	0.2091	0.2101	0.2103	0.2046	–	0.1150, 0.1227, 0.1237, 0.1239, 0.1182
	T_C	2.6872	6.9313	7.6933	7.7265	4.6889	10.8	10.8041, 18.3277, 19.5003, 19.6370, 14.0154
	α	0.1469	0.2656	0.2775	0.2777	0.2218	–	0.4443, 0.4570, 0.4585, 0.4586, 0.4510
	N_0V	0.2848	0.3572	0.3676	0.3681	0.3227	–	0.3660, 0.4418, 0.4527, 0.4540, 0.3997
$Mo_{0.60}Re_{0.40}$	λ	0.8627	1.1015	1.1392	1.1414	0.9797	0.86	0.8155, 1.0588, 1.0984, 1.1025, 0.9208
	μ^*	0.1950	0.2023	0.2032	0.2034	0.1980	–	0.1126, 0.1200, 0.1209, 0.1211, 0.1156
	T_C	7.5272	13.2687	14.1511	14.1902	10.4227	12.6	12.6061, 19.4510, 20.4785, 20.5741, 15.7183
	α	0.3217	0.3699	0.3751	0.3751	0.3515	–	0.4568, 0.4655, 0.4665, 0.4666, 0.4616
	N_0V	0.3741	0.4492	0.4597	0.4603	0.4134	–	0.4036, 0.4784, 0.4891, 0.4901, 0.4383
$Mo_{0.50}Re_{0.50}$	λ	0.9524	1.2145	1.2558	1.2581	1.0796	0.85	0.8007, 1.0329, 1.0703, 1.0736, 0.9044
	μ^*	0.1924	0.1994	0.2003	0.2005	0.1953	–	0.1115, 0.1186, 0.1196, 0.1197, 0.1144
	T_C	9.5387	15.3912	16.2568	16.2955	12.5123	11.5	11.5018, 17.7178, 18.6511, 18.7213, 14.4160
	α	0.3568	0.3926	0.3964	0.3965	0.3787	–	0.4567, 0.4653, 0.4663, 0.4663, 0.4616
	N_0V	0.3568	0.3926	0.3964	0.3965	0.3787	–	0.3989, 0.4715, 0.4819, 0.4827, 0.4336
$Mo_{0.50}Tc_{0.50}$	λ	1.5992	2.0375	2.1064	2.1103	1.8106	0.91	0.8611, 1.0821, 1.1143, 1.1157, 0.9763
	μ^*	0.1898	0.1966	0.1975	0.1976	0.1926	–	0.1104, 0.1174, 0.1183, 0.1185, 0.1132
	T_C	22.6121	28.4582	29.2355	29.2692	25.7115	12.6	12.6064, 17.9538, 18.6717, 18.6911, 15.5701
	α	0.4349	0.4454	0.4466	0.4466	0.4414	–	0.4622, 0.4682, 0.4688, 0.4688, 0.4665
	N_0V	0.5743	0.6454	0.6548	0.6553	0.6114	–	0.4211, 0.4863, 0.4948, 0.4951, 0.4572

TABLE III (cont.)

Alloys	SSP	Present result					Exp.	Theor. [3, 4]
		H	T	IU	F	S	[21]	
$Zr_{0.97}Rh_{0.03}$	λ	0.4501	0.6108	0.6392	0.6406	0.5493	0.59	0.5833, 0.8109, 0.8521, 0.8560, 0.7139
	μ^*	0.1957	0.2065	0.2079	0.2081	0.2020	–	0.1256, 0.1355, 0.1369, 0.1371, 0.1313
	T_C	0.0886	0.9882	1.2703	1.2812	0.5170	3.1	3.1000, 7.5696, 8.4111, 8.4845, 5.6233
	α	-0.4260	0.0368	0.0772	0.0778	-0.0682	–	0.3959, 0.4295, 0.4333, 0.4335, 0.4194
	N_0V	0.1805	0.2599	0.2727	0.2733	0.2316	–	0.2991, 0.3888, 0.4030, 0.4043, 0.3533
$Zr_{0.96}Rh_{0.04}$	λ	0.5238	0.7107	0.7437	0.7454	0.6392	0.64	0.6291, 0.8703, 0.9139, 0.9176, 0.7697
	μ^*	0.1928	0.2032	0.2046	0.2048	0.1989	–	0.1244, 0.1341, 0.1354, 0.1356, 0.1300
	T_C	0.4250	2.2067	2.6420	2.6588	1.3949	3.8	3.8008, 8.3216, 9.1388, 9.2006, 6.4424
	α	-0.0418	0.1967	0.2195	0.2198	0.1396	–	0.4125, 0.4389, 0.4419, 0.4421, 0.4312
	N_0V	0.2242	0.3082	0.3216	0.3222	0.2784	–	0.3211, 0.4110, 0.4252, 0.4263, 0.3763
$Zr_{0.95}Rh_{0.05}$	λ	0.6061	0.8222	0.8604	0.8623	0.7394	0.70	0.6931, 0.9556, 1.0030, 1.0067, 0.8476
	μ^*	0.1901	0.2002	0.2015	0.2018	0.1960	–	0.1232, 0.1327, 0.1340, 0.1343, 0.1287
	T_C	1.1362	3.7825	4.3324	4.3538	2.6841	4.8	4.8039, 9.4192, 10.2164, 10.2710, 7.5776
	α	0.1501	0.2877	0.3016	0.3018	0.2536	–	0.4285, 0.4485, 0.4508, 0.4509, 0.4428
	N_0V	0.2682	0.3559	0.3696	0.3702	0.3249	–	0.3496, 0.4403, 0.4545, 0.4555, 0.4060
$Zr_{0.94}Rh_{0.06}$	λ	0.6948	0.9424	0.9862	0.9884	0.8476	0.78	0.7592, 1.0433, 1.0945, 1.0982, 0.9280
	μ^*	0.1876	0.1974	0.1987	0.1990	0.1933	–	0.1221, 0.1315, 0.1328, 0.1330, 0.1275
	T_C	2.1652	5.4618	6.0769	6.1010	4.1764	5.75	5.7535, 10.3426, 11.1066 11.1539 8.5754
	α	0.2557	0.3425	0.3516	0.3517	0.3205	–	0.4403, 0.4557, 0.4576, 0.4576, 0.4514
	N_0V	0.3108	0.4012	0.4151	0.4158	0.3695	–	0.3769, 0.4680, 0.4821, 0.4830, 0.4342
$Zr_{0.93}Rh_{0.07}$	λ	0.7231	0.9806	1.0261	1.0285	0.8819	0.80	0.7757, 1.0645, 1.1164, 1.1201, 0.9479
	μ^*	0.1868	0.1966	0.1979	0.1981	0.1925	–	0.1218, 0.1311, 0.1324, 0.1326, 0.1272
	T_C	2.5221	5.9641	6.5901	6.6145	4.6416	5.85	5.9528, 10.4922, 11.2417, 11.2862, 8.7620
	α	0.2785	0.3549	0.3630	0.3631	0.3354	–	0.4428, 0.4573, 0.4590, 0.4591, 0.4533
	N_0V	0.3235	0.4144	0.4285	0.4291	0.3826	–	0.3835, 0.4744, 0.4884, 0.4893, 0.4409

Superconducting state parameters of the d-transition metals based binary alloys. T_C [K]. TABLE IV

Alloys	SSP	Present result					Exp.	Theor. [5]
		H	T	IU	F	S	[21]	
$Hf_{0.30}Ta_{0.70}$	λ	0.8297	1.0983	1.1439	1.1463	0.9859	0.82	0.7792, 1.0615, 1.1105, 1.1163, 0.9248
	μ^*	0.2047	0.2118	0.2127	0.2128	0.2085	–	0.1166, 0.1249, 0.1260, 0.1262, 0.1210
	T_C	3.7034	7.6222	8.2780	8.3066	6.0080	6.81	6.8109, 11.7232, 12.5031, 12.5901, 9.4420
	α	0.2765	0.3507	0.3585	0.3586	0.3288	–	0.4492, 0.4620, 0.4635, 0.4636, 0.4573
	N_0V	0.3563	0.4436	0.4565	0.4571	0.4100	–	0.38708, 0.4767, 0.4899, 0.4914, 0.4367
$Ta_{0.84}W_{0.16}$	λ	0.7054	0.9231	0.9593	0.9613	0.8270	0.51	0.5845, 0.7833, 0.8172, 0.8209, 0.6835
	μ^*	0.2116	0.2186	0.2195	0.2197	0.2151	–	0.1167, 0.1248, 0.1259, 0.1261, 0.1207
	T_C	2.2000	5.7908	6.4465	6.4758	4.1363	1.85, 3.80	3.8024, 8.2154, 8.9926, 9.0735, 5.9634
	α	0.1457	0.2762	0.2891	0.2894	0.2356	–	0.4156, 0.4399, 0.4427, 0.4429, 0.4306
	N_0V	0.3009	0.3831	0.3952	0.3958	0.3493	–	0.3055, 0.3846, 0.3966, 0.3979, 0.3471
$Ta_{0.60}W_{0.40}$	λ	0.6511	0.8494	0.8821	0.8839	0.7604	0.39	0.4883, 0.6493, 0.6766, 0.6793, 0.5689
	μ^*	0.2148	0.2219	0.2228	0.2229	0.2183	–	0.1170, 0.1252, 0.1262, 0.1264, 0.1210
	T_C	1.4785	4.6432	5.2593	5.2869	3.1052	2.00	2.0002, 5.3718, 6.0266, 6.0867, 3.5802
	α	0.0454	0.2229	0.2399	0.2403	0.1672	–	0.3776, 0.4160, 0.4203, 0.4205, 0.4016
	N_0V	0.2741	0.3541	0.3659	0.3665	0.3205	–	0.2571, 0.3296, 0.3408, 0.3418, 0.2952
$Ta_{0.40}W_{0.60}$	λ	0.5978	0.7779	0.8074	0.8090	0.6959	0.25	0.4121, 0.5444, 0.5667, 0.5687, 0.4789
	μ^*	0.2179	0.2251	0.2260	0.2262	0.2214	–	0.1174, 0.1256, 0.1267, 0.1269, 0.1214
	T_C	0.8463	3.4037	3.9474	3.9719	2.0820	0.85	0.8512, 3.0657, 3.5524, 3.5918, 1.8273
	α	-0.1040	0.1481	0.1714	0.1720	0.0691	–	0.3186, 0.3804, 0.3870, 0.3873, 0.3578
	N_0V	0.2462	0.3238	0.3353	0.3358	0.2906	–	0.2144, 0.2802, 0.2904, 0.2912, 0.2491
$Ta_{0.20}W_{0.80}$	λ	0.5207	0.6758	0.7012	0.7026	0.6043	0.26	0.3314, 0.4351, 0.4524, 0.4538, 0.3841
	μ^*	0.2224	0.2298	0.2307	0.2309	0.2259	–	0.1182, 0.1265, 0.1276, 0.1278, 0.1221
	T_C	0.2271	1.6746	2.0519	2.0691	0.8332	0.16	0.1601, 1.0621, 1.3125, 1.3301, 0.5049
	α	-0.5074	-0.0334	0.0072	0.0083	-0.1784	–	0.1733, 0.2988, 0.3116, 0.3120, 0.2550
	N_0V	0.2025	0.2763	0.2873	0.2879	0.2442	–	0.1638, 0.2211, 0.2302, 0.2308, 0.1942

TABLE IV (cont.)

Alloys	SSP	Present result					Exp.	Theor. [5]
		H	T	IU	F	S	[21]	
	λ	0.5016	0.6503	0.6745	0.6758	0.5813	0.27	0.2701, 0.3508, 0.3640, 0.3648, 0.3129
	μ^*	0.2238	0.2313	0.2322	0.2324	0.2274	–	0.1184, 0.1267, 0.1278, 0.1280, 0.1223
$Ta_{0.10}W_{0.90}$	T_C	0.1401	1.3072	1.6344	1.6493	0.5996	–	0.0113, 0.1998, 0.2718, 0.2749, 0.0712
	α	-0.6836	-0.1070	-0.0589	-0.0576	-0.2823	–	−0.1213 01449 01702 01703 0.0627
	N_0V	0.1908	0.2633	0.2742	0.2747	0.2315	–	0.1218, 0.1699, 0.1775, 0.1778, 0.1484
	λ	0.5047	0.6527	0.6768	0.6781	0.5831	0.32	0.3200, 0.4189, 0.4353, 0.4367, 0.3690
	μ^*	0.2246	0.2320	0.2329	0.2331	0.2281	–	0.1181, 0.1263, 0.1274, 0.1276, 0.1219
$W_{0.95}Re_{0.05}$	T_C	0.1511	1.3639	1.6997	1.7151	0.6239	–	0.1196, 0.8935, 1.1172, 1.1336, 0.3963
	α	-0.6772	-0.1080	-0.0604	-0.0592	-0.2847	–	0.1398, 0.2801, 0.2943, 0.2948, 0.2296
	N_0V	0.1920	0.2641	0.2748	0.2753	0.2320	–	0.1564, 0.2119, 0.2206, 0.2212, 0.1851
	λ	0.5189	0.6707	0.6953	0.6966	0.5990	0.38	0.3801, 0.5009, 0.5211, 0.5232, 0.4371
	μ^*	0.2241	0.2314	0.2323	0.2325	0.2275	–	0.1178, 0.1260, 0.1271, 0.1273, 0.1216
$W_{0.925}Re_{0.075}$	T_C	0.2164	1.6457	2.0205	2.0376	0.7934	–	0.5726, 2.4949, 2.9470, 2.9914, 1.3138
	α	-0.5574	-0.0598	-0.0175	-0.0163	-0.2168	–	0.2760, 0.3559, 0.3642, 0.3648, 0.3240
	N_0V	0.2003	0.2729	0.2836	0.2842	0.2405	–	0.1949, 0.2576, 0.2673, 0.2683, 0.2258
	λ	0.5344	0.6904	0.7156	0.7170	0.6165	0.42	0.3908, 0.5148, 0.5354, 0.5376, 0.4490
	μ^*	0.2235	0.2308	0.2317	0.2319	0.2269	–	0.1176, 0.1257, 0.1268, 0.1270, 0.1213
$W_{0.90}Re_{0.10}$	T_C	0.3062	1.9805	2.3968	2.4158	1.0048	0.70	0.7016, 2.8311, 3.3169, 3.3647, 1.5355
	α	-0.4463	-0.0134	0.0241	0.0251	-0.1520	–	0.2927, 0.3651, 0.3728, 0.3732, 0.3360
	N_0V	0.2092	0.2824	0.2932	0.2937	0.2497	–	0.2016, 0.2650, 0.2749, 0.2758, 0.2327
	λ	0.5815	0.7504	0.7777	0.7792	0.6699	0.50	0.4775, 0.6316, 0.6572, 0.6604, 0.5467
	μ^*	0.2218	0.2289	0.2297	0.2299	0.2250	–	0.1169, 0.1249, 0.1259, 0.1261, 0.1205
$W_{0.85}Re_{0.15}$	T_C	0.7044	3.1356	3.6674	3.6916	1.7971	2.26	2.2610, 6.1837, 6.9407, 7.0299, 3.8719
	α	-0.2029	0.0946	0.1216	0.1224	-0.0040	–	0.3721, 0.4121, 0.4165, 0.4169, 0.3947
	N_0V	0.2353	0.3101	0.3210	0.3215	0.2765	–	0.2515, 0.3219, 0.3326, 0.3338, 0.2847
	λ	0.6196	0.7988	0.8276	0.8292	0.7128	0.54	0.5162, 0.6825, 0.7101, 0.7136, 0.5897
	μ^*	0.2205	0.2275	0.2284	0.2285	0.2237	–	0.1163, 0.1242, 0.1253, 0.1255, 0.1199
$W_{0.80}Re_{0.20}$	T_C	1.1658	4.1891	4.8009	4.8288	2.5772	3.20	3.2032, 7.7802, 8.6182, 8.7196, 5.1097
	α	-0.0738	0.1558	0.1772	0.1778	0.0778	–	0.3930, 0.4248, 0.4283, 0.4287, 0.4106
	N_0V	0.2553	0.3309	0.3420	0.3425	0.2968	–	0.2722, 0.3445, 0.3554, 0.3567, 0.3059
	λ	0.6684	0.8607	0.8916	0.8933	0.7678	0.60	0.5693, 0.7526, 0.7829, 0.7868, 0.6489
	μ^*	0.2191	0.2259	0.2267	0.2269	0.2221	–	0.1157, 0.1235, 0.1245, 0.1247, 0.1192
$W_{0.75}Re_{0.25}$	T_C	1.9158	5.6217	6.3166	6.3484	3.7062	4.64	4.6438, 9.9703, 10.8923, 11.0077, 6.8903
	α	0.0420	0.2138	0.2303	0.2307	0.1540	–	0.4133, 0.4376, 0.4403, 0.4405, 0.4265
	N_0V	0.2795	0.3562	0.3672	0.3678	0.3214	–	0.2989, 0.3735, 0.3846, 0.3860, 0.3332
	λ	1.0934	1.3890	1.4352	1.4379	1.2329	0.70	0.6608, 0.8506, 0.8810, 0.8838, 0.7415
	μ^*	0.2115	0.2173	0.2180	0.2181	0.2138	–	0.1108, 0.1178, 0.1187, 0.1189, 0.1135
$W_{0.88}Re_{0.12}$	T_C	12.0103	18.3615	19.2694	19.3121	15.1772	7.47	7.4706, 12.9823, 13.8547, 13.9267, 9.8559
	α	0.3502	0.3874	0.3914	0.3915	0.3722	–	0.4413, 0.4546, 0.4562, 0.4562, 0.4486
	N_0V	0.4423	0.5179	0.5281	0.5287	0.4805	–	0.3436, 0.4132, 0.4233, 0.4241, 0.3751
	λ	0.7725	0.9862	1.0199	1.0218	0.8771	0.47	0.4351, 0.5603, 0.5805, 0.5821, 0.4929
	μ^*	0.2158	0.2221	0.2229	0.2230	0.2185	–	0.1130, 0.1204, 0.1213, 0.1215, 0.1160
$Re_{0.70}Os_{0.30}$	T_C	4.1465	9.0396	9.8509	9.8888	6.5076	1.45	1.4501, 4.1089, 4.6327, 4.6671, 2.5642
	α	0.1909	0.2921	0.3022	0.3024	0.2532	–	0.3578, 0.4000, 0.4047, 0.4048, 0.3830
	N_0V	0.3270	0.4029	0.4136	0.4141	0.3664	–	0.2308, 0.2915, 0.3006, 0.3012, 0.2603
	λ	0.3973	0.5137	0.5325	0.5336	0.4588	0.42	0.4200, 0.5619, 0.5854, 0.5891, 0.4802
	μ^*	0.2247	0.2321	0.2330	0.2332	0.2281	–	0.1180, 0.1263, 0.1273, 0.1275, 0.1218
$Re_{0.30}Os_{0.70}$	T_C	0.0011	0.1347	0.2049	0.2083	0.0279	–	1.1383, 4.1641, 4.8073, 4.9098, 2.2128
	α	-2.8229	-0.7952	-0.6609	-0.6571	-1.3454	–	0.3238, 0.3862, 0.3926, 0.3934, 0.3571
	N_0V	0.1268	0.1920	0.2018	0.2023	0.1628	–	0.2185, 0.2884, 0.2989, 0.3006, 0.2494

Here, the μ^* lies between 0.18 and 0.23 and is found quite higher in accordance with McMillan [21] for transition metals which may be due to the restriction of the band mass $m_b = 1$ of all alloying compounds for the sake of simplicity. The weak screening influences show on the computed values of the μ^*. The experimental data of the μ^* is not available for the further comparisons. But, we have compared our results with theoretical one [3–5] and found accordance with them.

The present results of T_C are found in good qualitative agreement with available experimental [21] and theoretical [3–5] data. The present results show a vast deviation with the available experimental data [21] and also are found in the range of experimental data [21] for some alloying compounds but those for another alloys, the present results are much higher than those. Also, the above observations indicate that the transition metals based binary alloys having high valence tend to have higher T_C due to unusually high Debye temperature except for some alloys, the T_C is lower. The higher or lower values of T_C can be due to the electron transfer between two metallic elements used in alloy construction. The increase and decrease in T_C has also been attributed to the excitonic mechanism resulting from the granular arrangement separated by semiconducting or insulating materials [2].

The computed values of the α show a weak dependence on the dielectric screening. Since the experimental value of α has not been reported in the literature so far, the present data of α may be used for the study of ionic vibrations in the superconductivity of alloying substances in connections with the available theoretical data [3–5]. Since H-local field correction function yields the comparable results of λ and T_C for most of the alloying complexes, it may be observed that α values obtained from this screening provide the best account for the role of the ionic vibrations in superconducting behaviour of these systems. The negative values of the α indicate that the electron–phonon coupling in these alloys does not fully explain all the features regarding their superconducting behavior because of the magnetic interactions of the atoms in alloys superconductors [38]. Hence, for alloys $A_{1-x}B_x$, where x is the concentration of the second metallic component, as the concentration of the B increases, the magnetic interactions of the atoms increase in metallic complexes. Also, the electron–lattice interactions are not deeply involved in such superconductors, which may cause the negative values of the isotope effect exponent α. Since the experimental value of α has not been reported in the literature so far, the present data may be used for the study of ionic vibrations in the superconductivity of binary alloys superconductors.

The magnitude of N_0V shows that the 4*d*- and 5*d*-transition metals based binary alloys under investigation lie in the range of weak to intermediate coupling superconductors. The values of the N_0V also show a feeble dependence on dielectric screening. The experimental data of the N_0V is not available for the further comparisons. But, it is found more comparable with available theoretical [3–5] yielding.

In general, one can see that among the five screening functions the screening function due to H (only static — without exchange and correlation) gives the minimum value of the SSP while the screening function due to F gives the maximum value. The present findings due to T, IU and S-local field correction functions are lying between these two screening functions. Hence, these local field correction functions are able to generate consistent results regarding the SSP of transition metals based binary alloys in comparison with more commonly employed H and T-functions. The data generated from IU- and F-function are seen with overlapping nature with almost each other. The effect of local field correction functions plays an important role in the computation of λ and μ^*, which makes drastic variation on T_C, α and N_0V. Thus, the use of these more promising local field correction functions is established successfully. Also, the presently computed data of the SSP lie within the theoretical limits of the Eliashberg–McMillan formulation.

According to the Matthias rules [25, 26], the binary alloys having $Z > 2$ i.e. 4*d*- and 5*d*-transition metal based binary alloys organize predictive superconducting nature. Also, one can go from $Z = 3.93$ to $Z = 6.5$ in 4*d*-alloys and $Z = 4.7$ to $Z = 6.88$, in 5*d*-alloys, the electron–phonon coupling strength λ varies with lattice spacing a. Related trends are also observed in the values of T_C for most of the binary alloys. Hence, a strong dependence of the superconducting transition temperature T_C of the 4*d*- and 5*d*-transition metals based binary alloys on the valence Z is found, which are displayed in Fig. 1 in accordance with the Matthias rules [25, 26].

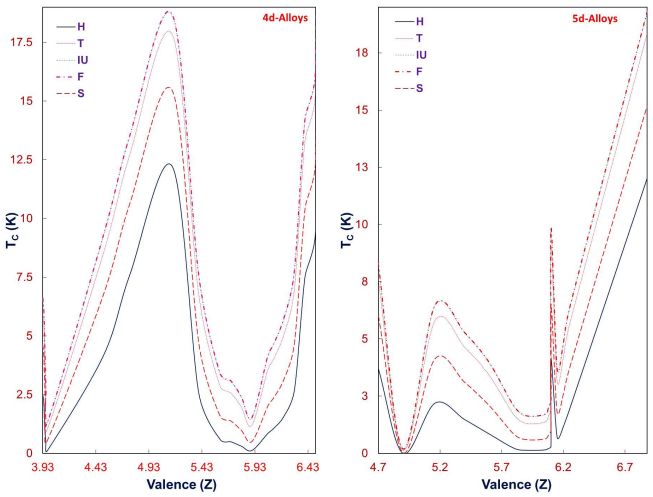

Fig. 1. Variation of transition temperature T_C with valence Z for (left) 4*d*- and (right) 5*d*-transition metals based binary alloys.

Finally, we would like to highlight the importance of the precise form for the model pseudopotential. It must be admitted that although the effect of model pseudopo-

tential in strong coupling superconductor is large, yet it plays a pivotal role in weak coupling superconductors i.e. those substances which are at the boundary dividing the superconducting and non-superconducting region. In other words, a small variation in the value of electron–ion interaction may lead to an abrupt change in the superconducting properties of the material under consideration. In this connection we may realize the importance of an accurate form for the model pseudopotential.

4. Conclusions

The comparison of presently computed results with available experimental and theoretical findings is highly promising in the case of transition metals based binary alloys, which confirms the usage of the model pseudopotential. The experimental values of most of the parameters are not available in the literature, hence, the comparison with other such theoretical data highly supports the present computations of the SSP.

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