

A LOCAL PSEUDOPOTENTIAL IN THE STUDY OF METALLIC PROPERTIES OF RHODIUM AND IRIDIUM

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A local pseudopotential has been proposed in this paper. This potential is used to calculate total energy, phonon dispersion curves (q-space and r-space), phonon density of states, Mode Grüneisen parameters, dynamic elastic constants, bulk modulus, maximum phonon frequency, mean phonon frequency, fundamental frequency (second moment of phonon frequency) and propagation velocities of elastic waves of rhodium and iridium. The contribution of d-like electron is taken into account by introducing repulsive short-range Born-Mayer term. A unique technique is suggested for the determination of the potential parameter which is independent of any fitting procedure and a new criterion for the selection of the exchange and correlation effects is also searched out by considering the minimization of total energy. A good agreement between theoretical investigations and experimental findings has confirmed our formulation.

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1 Introduction

During the last four decades a great interest has been shown to study the metallic properties of simple metals, but this technique has not been applied extensively to transition metals, particularly there have been few attempts for Rh and Ir during last two decades [1–17]. Rhodium and Iridium possesses unusual mechanical properties, which are characterized by brittle failure of single crystal at high pressure and at normal temperature [7]. Wills and Harrison [8] have calculated the elastic constants, bulk modulus and Grüneisen parameters of all transition metals using the Ashcroft's [8] empty core model potential in which the potential parameter is fitted with the experimental values of the bulk modulus at the equilibrium volume. Their theoretical results are found to deviate by 25%–55%. Cleri and Rosato [9] have used empirical many-body potential and calculated thermodynamic and structural properties of several transition metals. Their empirical potential is consist of four adjustable parameters, which they have fitted with the experimental values of the elastic constants. The theoretical investigations of Cleri and Rosato [9] have discrepancy of about 0–43% from the experimental findings. Soderlind et al. [10] have calculated the elastic constants using the local density approximation (LDA) with Full Potential Muffin Tin Orbital method, where input parameters are crystal structure and nuclear charge only. The variation observed in the theoretical investigation of Soderlind et al. is 0–43% from the experimental results. Wojciechowski [11] have calculated the bulk properties of Rh and Ir with

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the novel idea of metallic valence and their results are excellent. Cagin et al. [12] have calculated the thermal and elastic properties of these metals using the molecular dynamics (MD) simulation with Sutton-Chen [12] potential, which bears four adjustable parameters to be evaluated by fitting with the experimental values of elastic constants. The method adopted by Cagin et al. [12] is very sophisticated but it is also having the variation of about 15–28% from the observed values. Greenberg et al. [13] found that the contribution of three-body interactions to the lattice properties is very small for Ir. The Lattice dynamics, thermodynamics and equation of states of about ten transition elements including Rh and Ir have been studied by Antonov et al. [14] using their own model potential, which is having single parameter and evaluated by zero pressure condition. On the same way and with the same potential with little modification Ivanov et al. [7] have studied phonon spectra, inter atomic interaction and lattice defects of Rh and Ir. Recently, Singh [15] has theoretically investigated the phonon dispersion, phase stability and elastic constants of Rh and Ir by transition metal model potential (TMMP). They have used the effective value of TMPP. The result of Singh [15] has the variation up to 30% and it may be because they have taken the effective value of the pair potential through the Gaussian fitting. Recently Eicher et al. [16] have experimentally investigated phonon spectra of Rh in detail and have also reported the theoretical results using ab initio local density approximation (LDF). Their LDF calculations have been performed using ultrasoft pseudopotential and plane-wave basis norm-conserving pseudopotential with mixed bases set which include also all-electron calculations at a few high-symmetry points. This is most sophisticated and time consuming method. This method reproduces the phonon spectra excellently but having variation 0–12% in the calculation of the elastic constants. They were also successful in explaining Kohn anomalies in Rh [7]. Heid et al. [17] have reported the experimental results of phonon dispersion of Ir along major symmetry directions.

From the above study we have seen that even with the experimental input many [8–10,12,15] theories failed to reproduce the results of the metallic properties of transition metals. Even the most sophisticated methods [12,16] could not avoid reasonable deviation from the experimental findings. Moreover, it is also seen that the same set of potential and its parameter did not explain all the properties of metallic system with the same accuracy. Keeping all these things in mind we have proposed a simple form of pseudopotential having unique way of determining of its parameter. We have also put forward a meaningful criterion for the selection of exchange and correlation effects. This is free from any fitting procedure and independent of any experimental observation. Using this potential, in the present paper, we have calculated the total energy, phonon dispersion curves (\mathbf{q} -space and \mathbf{r} -space analysis), phonon density of states, Mode Grüneisen parameters, dynamic elastic constants, bulk modulus, maximum phonon frequency, mean phonon frequency, fundamental frequency (second moment of phonon frequency) and propagation velocities of elastic waves of Rh and Ir.

2 A Model Potential

In every pseudopotential formalism either local or nonlocal approach has been used for the calculation of metallic properties [18–22]. A nonlocal pseudopotential is complicated to tackle so most of the people preferred to work on logically acceptable local pseudopotential. In the present article we have proposed a local form of pseudopotential, which includes in a simple parametric way all the features dictated by the physics of the situation. Particularly it is seen that in noble,

transition and actinide metals, below the Fermi energy level there are filled d- and f-bands which tend to push up the energy of a given state. Hence, effect called “hybridization” would require a repulsive term in the model potential. Hence, in r-space, inside the core radius, the model potential is combination of repulsive and attractive interactions (i.e. varying cancellation within the core). Beyond the core radius, the model potential is Coulombic in nature. In real space the potential (in Ryd.) has the following form

$$\begin{aligned} W(r) &= -\frac{2Z}{r_c^2} \left[2 - \exp\left(1 - \frac{r}{r_c}\right) \right] r, & r < r_c \\ &= -\frac{2Z}{r}, & r \geq r_c \end{aligned} \quad (1)$$

In the wave number space (\mathbf{q} -space) the potential takes the form as (in Ryd.)

$$W_B(q) = -\frac{8\pi Z}{\Omega_0 q^2} \left\{ \begin{aligned} &\frac{4(\cos(qr_c) - 1)}{q^2 r_c^2} + \frac{4 \sin(qr_c)}{qr_c} + \frac{\sin(qr_c)}{(1 + q^2 r_c^2)^3} [5qr_c - 4q^3 r_c^3 - q^5 r_c^5] \\ &+ \frac{\cos(qr_c)}{(1 + q^2 r_c^2)^3} [11q^2 r_c^2 + 4q^4 r_c^4 + q^6 r_c^6] + \frac{2eq^2 r_c^2 (q^2 r_c^2 - 3)}{(1 + q^2 r_c^2)^3} - \cos(qr_c) \end{aligned} \right\}, \quad (2)$$

where Z is the valency, Ω_0 the volume per ion, \mathbf{q} the wave vector and e the base of natural logarithm. It is evident that the potential contains only one parameter r_c . In addition, the potential is continuous at $r = r_c$ and its strength goes on decreasing as $r \rightarrow 0$ within the core. Which is essential requirement of pseudopotential formalism. It is also found that screened form factor $W(q)$ does not show any predominating oscillatory behavior at large value of q , which is also an important feature in characterizing the form factor.

3 Determination of potential parameter

In the literature survey [18–29] we found that the practical usefulness of a unique method of determination of pseudopotential parameter has not been pointed out anywhere. People [18,25,26,28] have used values of ionic radii (core radii) Wigner-Seitz radii as the parameter of the potential. Many authors [8–10,12,23,24,26,29] have used different experimental input to determine the potential parameter viz., liquid metal resistivity, elastic constants, band gap at definite point in the Brillouin zone, phonon frequencies at some symmetry points in the Brillouin zone etc. Out of these the experimental input for band gap is not appropriate as Hamiltonian matrix is truncated after a few reciprocal lattice vectors. While in the phonon frequencies, it spans almost in entire range of $W(q)$ and at the same time energy calculation also requires $W(q)$ for large number of values of q . Many people [7,14] used zero pressure condition, which is equally important otherwise the properties will be determined at some non-zero volume strain. That is why the parameter of the potential should be determined in such a way that it captures almost entire range of q . Earlier, Heine and Wearie [30] have proposed a relation for the determination of the potential parameter, which depends on R_a (atomic radius) and Z (valence). They have considered the constant value of $q_0/2k_F$ and it is equal to 0.8 within the elements having $Z=1$ to $Z=8$ which is highly undesirable. It is also well known that the wave vector q_0 where the form

factor becomes zero first time plays vital role and its correct determination is extremely important [31,32]. Previously Jani and Patel [32] from our group had also proposed a quantum number dependency to determine the parameter of the potential. Cohen and Heine [33] has narrated the importance of quantum number ' l ' in the pseudopotential calculations from the repulsive centrifugal barrier $l(l+1)/r^2$ which occurs in the radial part of Schrödinger equation. If we attend all these features in the determination of potential parameter it is evident that parameter should possess Z_A (atomic number), R_a (Wigner-Seitz radius) and $l(l+1)$ dependency. Hence on the line of earlier work, we put efforts to search out a possible expression for the identification of the parameter. This is accomplished by making the parameter l , R_a , and Z_A dependent in the following simple way

$$r_c = l(l+1) \frac{R_a}{Z_A}, \quad (3)$$

where l , R_a and Z_A are orbital angular momentum quantum number (last ' l ' value of the filled shell for the respective element), atomic radius and atomic number, respectively. It may be noted that there are chances for redefining such relation in due course of time. This is an attempt to indicate the dependency of the r_c on certain aspect of the periodic table so that the behavior of the pseudopotential could be judged through out the periodic table. The above relation is used to evaluate the q_0 values for several elements. It is found from Tab. 1 that our q_0 values are very close to experimental findings and highly satisfactory. We feel here that as within the core there is varying cancellation and potential is l -dependent; it takes non-local character of the potential up to certain extent. This criterion leads the values of $r_c = 1.2474$ (a.u.) and $r_c = 1.1048$ (a.u.) for rhodium and iridium, respectively.

4 Selection of screening function from total energy calculation

There have been number of dielectric functions [18,34–42] tried to obtain the screened form factor of pseudopotential but there is no unique way of selecting proper screening function. It is well known that Taylor [34] screening function is best justified at high densities while Vashishta and Singwi [36] screening function at low densities. Ichimaru and Utsumi [37] screening function reproduces accurately the Monte Carlo results as well as those of microscopic calculations. It also satisfies self-consistency conditions in the compressibility sum rule and short-range correlations. A notable feature in this function is its involvement of the logarithmic singularity at $q = 2k_F$ and the accompanying peak at $q = 1.94k_F$. The Sarkar et al [38] screening function is also derived in the same fashion as that of the Ichimaru and Utsumi [37] and it is latest one.

The total energy of a crystal in the framework of second order perturbation treatment based on pseudopotential is given by [14]

$$E_{tot} = E_i + E_0 + E_1 + E_2 + \Phi_{sr}, \quad (4)$$

where $E_i = \alpha Z^2/r_a$, α is Madelung constant having the value 1.79175 for fcc structure.

$$E_0 = Z \left[\frac{2.21}{r_s^2} - \frac{0.916}{r_s} - 0.115 + 0.031 \ln(r_s) \right] \quad (5)$$

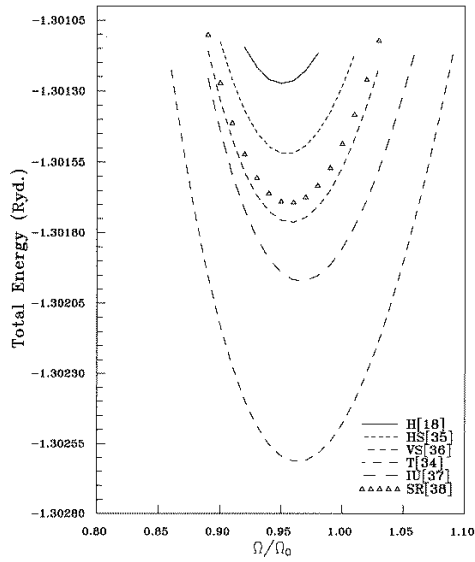


Fig. 1. Energy Volume relation for Rhodium.

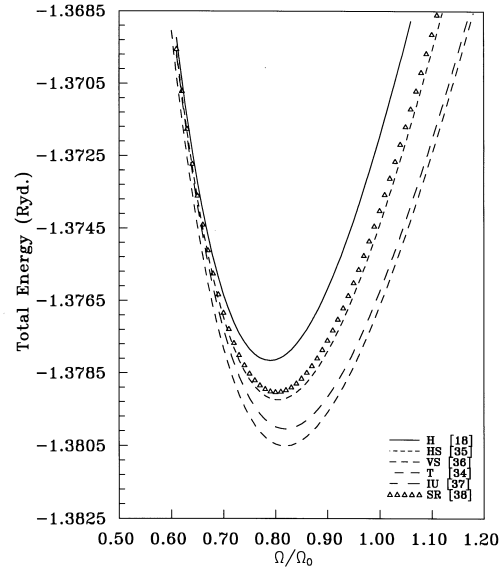


Fig. 2. Energy Volume relation for Iridium.

is the energy of a free electron gas, which is the sum of the kinetic, exchange and correlation energies.

$$E_1 = \lim_{q \rightarrow 0} \left[\frac{8\pi Z^2}{\Omega_0 q^2} + ZW_B(q) \right] \quad (6)$$

is the average energy of the electron-ion interaction. With our model potential it becomes

$$E_1 = \frac{8Zr_c^2 k_F^3}{3\pi} [6 \exp(+1) - 16], \quad (7)$$

where r_c is the parameter of the potential.

$$E_2 = \frac{\Omega_0}{16\pi} \sum' q^2 |W_B(q)|^2 \frac{\varepsilon_H(q)}{\{1 + [\varepsilon_H(q) - 1][1 - f(q)]\}} \quad (8)$$

The prime on the summation sign excludes the $q = 0$ term. Summation over 32 nearest neighbors in reciprocal space is taken to achieve proper convergence in fcc phase. The function $\varepsilon_H(q)$ is the Hartree static dielectric function and $f(q)$ incorporates the exchange and correlation effects.

The d-like contribution is added by [14]

$$\Phi_{sr} = 0.5A \sum_R \exp(-\alpha_B R), \quad (9)$$

which is known as the Born-Mayer potential and is valid for interaction of overlapping wave functions in atomic limit.

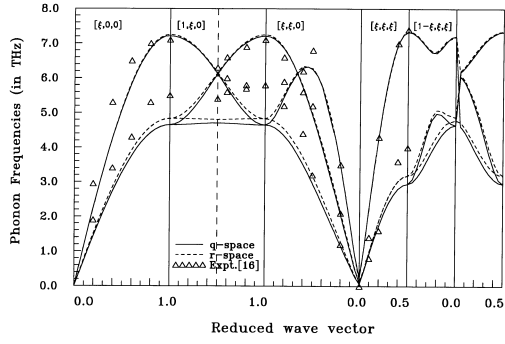


Fig. 3. Phonon dispersion curves for Rhodium.

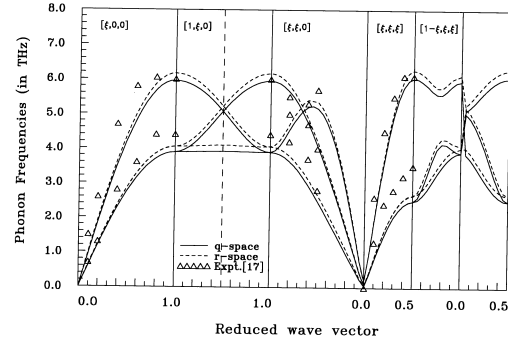


Fig. 4. Phonon dispersion curves for Iridium.

We have calculated the total energy of Rh and Ir using different screening functions, which is shown in Tab. 2 (at observed volume) and also the energy-volume relations which are shown in Figs. 1 and 2. For both the metals Taylor [34] screening function gives the lowest energy. Then the particular combination of screening function and r_c evaluated from equation (3) is used for the further calculation.

5 Phonon Dispersion curves (q-space and r-space)

The dynamical matrix from which phonon energies and polarization vectors are calculated may be obtained either by summing real-space force constants or by performing a sum in reciprocal space. It is known that the real space sum converges faster than the more common reciprocal space sum and is more justifiable for the calculation of thermal properties and integral properties of the electron-phonon interactions. We have used both the methods i.e. reciprocal space sum method as well as real space sum method for calculating the phonon dispersion relation of Rh and Ir using our model potential.

Computations of the phonon frequencies along the three principal symmetry directions of the reciprocal lattice namely the $(0, 0, \xi)$, $(0, \xi, \xi)$ and (ξ, ξ, ξ) directions have been carried out. In addition, we have also included the $(1, \xi, 0)$ and $(1 - \xi, \xi, \xi)$ directions in the present investigations. The secular determinant in \mathbf{q} -space has been solved for 50 nearest neighbors [43] while in \mathbf{r} -space it has been solved for 32 nearest neighbors [44,45].

The calculated phonon dispersion curves in \mathbf{q} -space and \mathbf{r} -space are compared with the experimental results of Eichler et al. [16] for Rh and Heid et al. [17] for Ir which are shown in Figs. 3 and 4 respectively. The discrepancies between theoretical findings and experimental results near Brillouin Zone (BZ) boundary in percentage are expressed in Tab. 3. The calculated values of phonon frequencies at (ξ, ξ, ξ) T branches near BZ boundary overestimate the experimental phonon frequencies at the maximum by 20% (r-space) and 26% (q-space) for Rh and that of 24% (r-space) and 28% (q-space) for Ir. The calculation of Singh [15] shows the discrepancies of 30% and 34% along the longitudinal branches at $(\xi, 0, 0)$ BZ boundary, while for (ξ, ξ, ξ) T mode near the BZ boundary the discrepancies are found as much as 22% and 19% for Rh and Ir respectively. Moreover he has not reported the phonon dispersion curves in the high symmetry

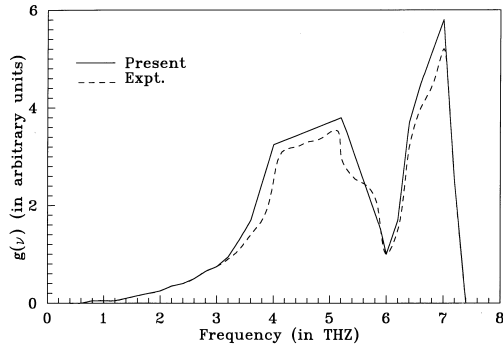


Fig. 5. Density of States (DOS) for Rhodium.

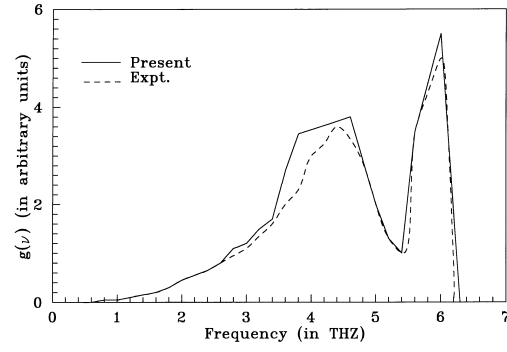


Fig. 6. Density of States (DOS) for Iridium.

direction viz. $(1, \xi, 0)$, $(1 - \xi, \xi, \xi)$. The deviation found in the calculation of phonon frequencies of Rh and Ir by Antonov et al. [14] is at $(\xi, 0, 0)$ BZ boundary for transverse mode it is 17% and 6% and for longitudinal mode it is 5% and 19% while for (ξ, ξ, ξ) T mode near the BZ boundary it is 49% and 33%. The results of Ivanov et al. [7] about phonon dispersion curves are deviated by 5% more than the deviation reported by Singh [15] for both Rh and Ir except (ξ, ξ, ξ) T mode near the BZ boundary.

Nevertheless previous model investigations [7,14,15] predicted even more overestimated values of the phonon frequencies at the BZ boundary. These discrepancies in the phonon frequencies could have been reduced by an adjustment of the model parameter but we preferred to leave it as such because the aim of the present work is to use an interatomic potential independent of any fitting through experimental frequencies.

6 Phonon Density of States (DOS)

The density of states i.e. frequency distribution curves are generated using a standard technique [46]. Our results of DOS show good agreement with experimental findings and are shown in figures 5 and 6 respectively for Rh and Ir.

7 Mode Grüneisen Parameters

The mode Grüneisen parameter $\gamma(\mathbf{q}, j)$ describes the change in the frequency $\omega(\mathbf{q}, j)$ of the phonon of wave vector \mathbf{q} and the branch index j with volume Ω and is defined by

$$\gamma(q,j) = -\frac{d[\ln\omega(q,j)]}{d[\ln\Omega]} \quad (10)$$

Figs. 7 and 8 display the mode Grüneisen parameters as calculated presently in the high symmetry directions. To the best of our knowledge, the mode Grüneisen parameters of Rh and Ir have not been measured. The experimental data, based on tunneling spectroscopy, indicates that the Grüneisen parameter is necessarily mode dependent and that the transverse modes are

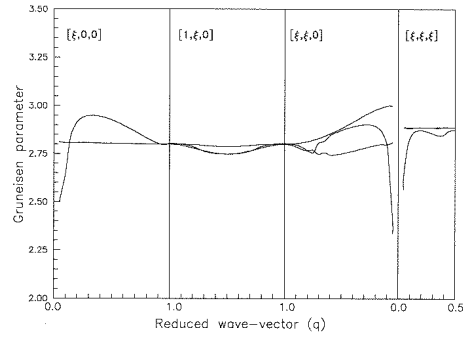


Fig. 7. Mode Grüneisen parameters for Rhodium.

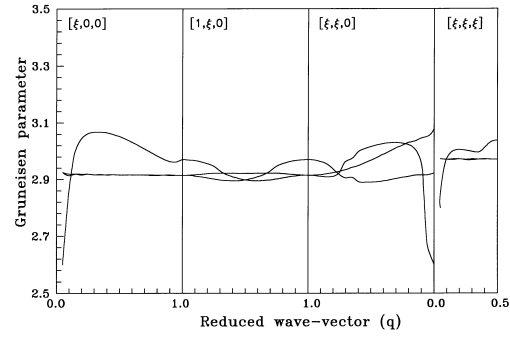


Fig. 8. Mode Grüneisen parameters for Iridium.

Metal	r_c (a.u.)	$q_0/2k_F$ Present Work	$q_0/2k_F$ Other values [18]
Li	1.8812	0.92	0.67, 0.77, 1.13, 1.26
Na	2.0530	1.02	0.866, 0.89, 0.96, 0.97, 0.98, 0.99
K	2.7322	0.94	0.93, 0.94
Rb	2.7017	1.02	0.78, 0.82, 0.94, 1.0
Cs	2.9375	1.02	0.79, 1.07
Cu	1.2128	1.22	1.36, 0.62
Ag	1.3931	1.20	1.52, 0.60
Au	1.3130	1.27	1.52, 0.60
Mg	1.6694	0.84	0.75, 0.78, 0.83, 0.90
Zn	1.2962	0.94	0.78, 0.83, 0.85, 0.87, 0.95
Hg	1.4516	0.97	0.67, 0.88, 0.92, 0.93, 1.19
Al	1.4335	0.77	0.73, 0.75, 0.76
Ga	1.3875	0.84	0.876, 0.916, 0.899, 0.944
In	1.5684	0.81	0.75, 0.83, 0.88, 0.90, 0.931, 0.956
Sn	1.5708	0.75	0.77, 0.83, 0.846
Pb	1.5606	0.78	0.64, 0.84, 0.88, 0.92
Si	1.3615	0.78	0.785, 0.884
Ge	1.2410	0.89	0.86, 0.883, 0.85, 0.847
Rh	1.2474	0.82	-
Ir	1.1048	0.86	-

Tab. 1. The potential parameter r_c (a.u.) and wave vector $q_0/2k_F$

more sensitive to the compression than the longitudinal one. The presently investigated values of mode Grüneisen parameter are comparable to those obtained by Antonov et al. [14].

Metal	Energy (Ryd.)					
	Hartree [18]	Taylor [34]	Hubbard- Sham [35]	Vashishta- Singwi [36]	Ichimaru- Utsumi [37]	Sarkar et al [38]
Rh	-1.3009	-1.3024	-1.3012	-1.3016	-1.3018	-1.3014
Ir	-1.3719	-1.3766	-1.3732	-1.3745	-1.3762	-1.3740

Tab. 2. Lowest energies for Rh and Ir using different screening functions at observed volume.

At BZ boundary	Rh			Ir		
	r-space	q-space	Expt. [16]	r-space	q-space	Expt. [17]
(1, ξ , 0)L	7.25(2)	7.21(1.5)	7.1	6.16(2)	5.95(0.8)	6.0
(ξ , ξ , ξ)L	7.35(0.6)	7.33(0.9)	7.4	6.27(2.7)	6.04(0.9)	6.1
(1 - ξ , ξ , ξ)L	7.1(4)	7.1(4)	6.8	6.00(1.6)	6.0(1.6)	5.9
(1, ξ , 0)T	4.83(12)	4.65(15)	5.5	4.05(7)	3.89(11)	4.4
(ξ , ξ , ξ)T	3.19(20)	2.95(26)	4.0	2.66(24)	2.49(28)	3.5
(1 - ξ , ξ , ξ)T	4.83(10)	4.65(4)	5.4	4.1(8)	4.0(11)	4.5

Tab. 3. The values of the phonon frequencies at the BZ boundary in q-space and r-space. (The value in the parenthesis gives the deviation from experimental value in percentage.)

8 Dynamical elastic constants and propagation velocities of elastic waves

The presently obtained values of the dynamical elastic constants C_{11} , C_{12} , C_{44} and bulk modulus are given in the Tabs. 4 and 5. The calculated results of C_{11} , C_{12} , C_{44} and bulk modulus deviate by 0%, 11.16%, 8%, 10%, for Rh and 3%, 13.9%, 20%, 4% for Ir from the experimental findings, respectively. The theoretical investigations reported by others [4,5,8,9,15] are varying from 0–54% for Rh and 3–49% for Ir. The propagation velocities of the elastic waves displayed in Ttab. 6 for Rh and Ir show excellent agreement with the experimental results.

9 The calculation ω_{\max} , $\langle\omega\rangle$, $\langle\omega^2\rangle^{1/2}$ and fundamental frequency $\langle\omega^2\rangle$

The quantities ω_{\max} , $\langle\omega\rangle$, $\langle\omega^2\rangle^{1/2}$ represents the main numerical characteristics of the density of the phonon states. The presently calculated value of ω_{\max} , $\langle\omega\rangle$, $\langle\omega^2\rangle^{1/2}$ are compared with the experimental [14] as well as other such theoretical findings [14] and are shown in Tab. 7. Our results shows good agreement with the experimental finding in general and also shows the superiority over the reported values of Antonov et al. [14] particularly for Ir. In the same table we have displayed the value of second moment i.e. fundamental frequency by adopting a way of Hartmann and Milbrodt [43]. To the best of our knowledge so far no one has reported the value of second moment for Rh and Ir.

	Present Work	Expt. [15]	Others						
			[15]	[8]	[15]	[5]	[4]	[9]	[16]
C ₁₁	4.16 (0)	4.16	2.88 (30)	3.14 (25)	3.27 (21)	5.55 (33)	3.97 (5)	3.92 (6)	4.022 (3)
C ₁₂	2.19 (11.16)	1.97	2.12 (8)	2.49 (26)	2.21 (12)	3.04 (54)	1.70 (13)	2.37 (20)	1.964 (1)
C ₄₄	1.99 (8)	1.84	1.84 (0)	1.28 (30)	1.05 (43)	2.09 (13)	1.96 (6)	1.99 (8)	1.622 (12)
C ₁₂ /C ₄₄	1.10	1.07	1.15	1.95	2.11	1.46	0.87	1.19	1.029
B	2.84 (10)	2.70	2.38 (12)	1.22 (55)	2.55 (5)	3.88 (43)	2.46 (9)	2.89 (6)	2.65 (2)

Tab. 4. Dynamical elastic constants and Bulk modulus of Rhodium. (The value in the parenthesis gives the deviation from experimental value in percentage.)

	Present Work	Expt. [15]	Others						
			[15]	[8]	[15]	[5]	[4]	[9]	[17]
C ₁₁	6.020 (3)	5.82	4.20 (28)	4.17 (28)	4.13 (29)	6.31 (8)	6.20 (6)	5.54 (5)	6.67 (15)
C ₁₂	2.074 (13.9)	2.41	3.02 (25)	3.24 (34)	2.76 (15)	3.12 (29)	2.65 (9)	3.45 (43)	2.82 (17)
C ₄₄	2.086 (20)	2.62	2.55 (3)	1.75 (33)	1.32 (49)	2.47 (5)	2.66 (1.5)	2.61 (0)	2.55 (3)
C ₁₂ /C ₄₄	0.994	0.919	1.18	1.86	2.09	1.27	1.00	1.32	1.11
B	3.389 (4)	3.55	3.42 (4)	1.80 (49)	3.23 (9)	4.19 (18)	3.83 (7)	4.15 (17)	4.11 (16)

Tab. 5. Dynamical elastic constants and Bulk modulus of Iridium. (The value in the parenthesis gives the deviation from experimental value in percentage.)

10 Conclusions

In order to interpret the results of complex structure of transition metals, rare earth metals, actinides and noble metals it is desirable to have simple method of general applicability, which can reproduce the results of most of physical properties very close to the experimental findings. The minimum energy criterion to select the screening function generates the interactions for the system in equilibrium while the l , R_a , and Z_A dependency of the parameter sense the non local character of the system which is essential for non simple, transition, alkaline earth, actinides etc., elements.

The results so obtained are also comparable to those obtained from the most sophisticated methods, which are intricate and require lengthy calculations with large computer time. The approach we suggest is simpler and less time consuming. Thus, the method can readily be used for the relative ease and accuracy.

Further, the earlier applications of model potentials were limited to fitting with experimental phonon frequencies at some symmetry points in the Brillouin zone. Moreover, the earlier reports do not identify a proper criterion about the choice of a screening function used.

In the light of the above facts, the successful application of present study confirms the formalism of the pseudopotential developed in the present work. From the success of our results we believe that it would be interesting to analyze all the model potentials reported so far on the line of the above criterion for the selection of screening function, which leads to the best result.

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	Rhodium		Iridium	
	Present Work	Expt.*	Present Work	Expt.*
v_l (100)	1.827	1.827	1.633	1.606
v_t (100)	1.264	1.215	0.961	1.077
v_l (110)	2.036	1.984	1.649	1.728
v_{t1} (110)	1.264	1.215	0.961	1.077
v_{t2} (110)	0.889	0.937	0.935	0.869
v_l (111)	2.101	2.034	1.654	1.766
v_t (111)	1.029	1.038	0.944	0.944

Tab. 6. Propagation velocities [in 10^5 cm/sec] of elastic waves of rhodium and iridium. (* estimated from the experimental data of elastic constants.)

Elements	ω_{\max}				$\langle\omega\rangle$			
	Present		Others [14]	Expt. [14]	Present		Others [14]	Expt. [14]
	q-space	r-space			q-space	r-space		
Rh	48.31	48.21	47.76	47.93	28.11	28.90	30.20	29.29
Ir	43.77	44.24	47.51	43.38	29.90	30.22	30.24	30.78
Elements	$\langle\omega^2\rangle^{1/2}$				$\langle\omega^2\rangle$			
	Present		Others [14]	Expt. [14]	Present	Others	Expt.	
	q-space	r-space						
Rh	27.64	28.04	28.22	28.13	8.16	-	-	
Ir	27.95	28.29	29.87	28.26	5.65	-	-	

Tab. 7. Comparison of maximum phonon frequency ω_{\max} (THZ) mean phonon frequency $\langle\omega\rangle$ (THZ), mean phonon frequency $\langle\omega^2\rangle^{1/2}$ (THZ) and Second moment (fundamental frequency) in (10^{25} rad/sec).

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