CHAPTER 2

Pseudopotential and Screening functions

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CHAPTER 2

2.1 Introduction

The Pseudopotential method is one of the simplest tools to study various physical and chemical properties of materials. The concept of pseudopotential has been developed within the ‘one electron model’, appears at first sight artificial and inconsistent. In the one electron model “each electron is considered separately as moving in the average field of nuclei and all the other electrons” [2.1].

The interaction potential between an atom and an electron with its Coulomb singularity at the nucleus may be replaced with a weak non singular potential without the electron so much as noticing the change which is known as the PSEUDOPOTENTIAL. Thus the Pseudopotential is the net effective weak potential in the neighbourhood of the ion core seen by an electron [2.1-2.6]. Pseudopotential is a system of ideas stemming from the fact that a short range “compensatory” term may be added to the electron – ion interaction potential which will model the combined action of the nucleus and the core electrons while leaving unchanged the long range part of the potential [2.2-2.6]. An original potential may be modified by adding a more or less arbitrary potential, but from the scattering theory point of view it will remain the same and it does not change the Eigen values of the Schrödinger equation.

In general, the pseudopotential is defined as “The fictitious / artificial but physically justifiable weak and effective potential seen by an electron in the vicinity of ions and the clouds of surrounding electrons” [2.1-2.3]. The term pseudopotential was first time used by Fermi [2.7] in the theory of low energy nucleon – nucleon scattering. Hellmann [2.8] applied it to atoms, in Solid State Physics, Phillips and Kleinmann [2.9] and Antonick [2.10] used this theory in study of energy band structure of semiconductors.

Pseudopotential is constructed in two different ways. One, the true atomic potential and the corresponding core wave functions have to be included explicitly. Second, the pseudopotential is replaced by a model potential having a simple
analytical or empirical form. The model pseudopotential is also called local pseudopotential, if it depends on the ion positions. It is called nonlocal, if it depends on the energy/momentum also. As non-local pseudopotentials are energy Eigen value dependent, the exact form of pseudopotential is quite difficult to implement in actual computational programs. Hence many people prefer to use local model potentials for the simplicity in the computations.

2.2 Concept of Pseudopotential

Physically, the cancellation between the true attractive potential and the repulsive orthogonalization term may be viewed as a manifestation of the Pauli exclusion principle, which, in the context, requires the valence electron function to be orthogonal to the occupied atomic core orbitals. The requirement of orthogonality manifests itself through the rapid oscillations of the true wave function in the ion-core region where the true potential is deep and attractive. Such rapid oscillations give rise to high kinetic energy of the valence electron, which act like a repulsive potential in the ion core region. As a result, the valence electron appears to see only a net weak potential called the Pseudopotential shown in figure 2.1. In the model potential method the true potential $V(r)$ within a sphere surrounding each ion is replaced by a flat potential $W(r)$, adjusted such that the model wave function $\phi$ has the same slope and derivative at the sphere surface as the true wave function $\psi$ but with nodes within the sphere eliminated.

The theoretical survey suggests that the concept of Pseudopotential is one of the methods to deal with the Schrödinger equation, which contains the essential feature of the behaviour of electrons in metallic system and easily understood by using orthogonalized plane wave (OPW) of wave number of $k$ [2.1-2.4]

\[ |OPW_{k}⟩ = (1 − p)|\bar{k}⟩. \]  

(2.1)

Where $|p⟩ = \sum_\alpha |\alpha⟩\langle\alpha|$ is the projection operator, in which $|\alpha⟩ = \psi_\alpha(r)$ presents a core state.
We may expand the conduction-band state in terms of general linear combination of OPW’s:

$$\psi_k = \sum_q a_q (\vec{k})(1 - P) |\vec{k} + \vec{q}\rangle.$$  \hfill (2.2) 

Let us assume

$$\phi_k = \sum a_q (\vec{k}) |\vec{k} + \vec{q}\rangle$$  \hfill (2.3) 

$$\therefore \psi_k = (1 - P)\phi_k.$$  \hfill (2.4) 

If we use this expansion in the Schrödinger equation 

$$H\psi_k = E(\vec{k})\psi_k,$$  \hfill (2.5) 

then we have

$$H(1 - P)\phi_k = E(\vec{k})(1 - P)\phi_k.$$
\[ T \phi_k + \left[ V(\vec{r}) - H + E(\vec{k})P \right] \phi_k = E(\vec{k}) \phi_k \]  

(2.6)

Where

\[ W(\vec{r}) = V(\vec{r}) + \left[ E(\vec{k}) - H \right] \]  

(2.7)

\[ = V(r) + \sum_{\alpha} [E(\vec{k}) - E_{\alpha}] \langle \alpha \rangle \langle \alpha \rangle \]

is known as the Pseudopotential and \( \phi_k \) is known as the pseudowavefunction.

Here in equation (2.7), the second term on the right is repulsive, since the dominant contribution comes out from the outer region of both the core orbitals, so that the difference \( E(\vec{k}) - E_{\alpha} \) will be positive. The first term due to the true potential felt by the valence electron in the core region of ions is actually strong and attractive. Thus the repulsive contribution cancels the true potential such that the pseudopotential becomes effectively weak [2.1-2.4]

An electron at any point \( \vec{r} \) will interact with all ions situated at the lattice site \( \vec{r}_i \) and so it is assumed to write pseudopotential \( W(\vec{r}) \) as the sum or superposition of the spherically symmetric individual ion pseudopotential. Thus,

\[ W(\vec{r}) = \sum_i w(\mid \vec{r} - \vec{r}_i \mid) \]  

(2.8)

Hence matrix element of the pseudopotential can be written as:

\[ \langle \vec{k} \mid W(\vec{r}) \mid \vec{k} \rangle = \frac{1}{\Omega} \int \exp(i\vec{k} \cdot \vec{r}) \sum w(\mid \vec{r} - \vec{r}_i \mid) \exp(-ik \cdot r) d^3r. \]  

(2.9)

\[ = S(q)W(q). \]
Here we have denoted \( q = k' - k \) and introduced the structure factor \( S(q) \) and the form factors of the single-site potential \( W(q) \).

\[
S(q) = \frac{1}{N} \sum \exp(-i q \cdot r_i).
\] (2.10)

\[
W(q) = \langle k + q | W | k \rangle = \frac{1}{\Omega} \int \exp[-i(\tilde{k} + q) \tilde{r}] W(\tilde{r}) \exp(i \tilde{k} \cdot \tilde{r}) d^3 \tilde{r}
\] (2.11)

The potential \( W(q) \) may be either local or non-local.

It is true that non-local pseudopotentials are to be preferred for accurate prediction of the properties of real materials, but the results properly generated by local pseudopotentials are also acceptable with tolerable errors. Local potential are conceptually and computationally simple. A large number of attempts dealing with the construction and applications of local model pseudopotentials are found in the literature and still people preferring to work with local pseudopotentials.

### 2.3 Concept of Screening

In the theory of metals the assembly of free electrons in the metals is considered as degenerate electron gas with uniform distribution. When an external positive charge is placed in such a system the whole distribution of electrons (density) changes so as to oppose the change in the potential or to maintain the equilibrium. This phenomenon is known as screening of positive charge. Due to screening effects the potential experienced by conduction electrons changes by a large amount. Also, the total displaced charge is equal to charge of the ion \([2.11, 2.12]\).

Screening plays very important role in the response of metals to any external field. In order to calculate the effect of screening we need to divide each Fourier component of bare ion potential by dielectric screening function \([2.12, 2.13]\).

\[
V_s(q) = \frac{V_b(q)}{\epsilon(q)}
\] (2.12)
Initially, only static dielectric function was introduced in which direct electron–
electron interactions were not included. It was termed as static Hartree dielectric
function [2.13]. After that it was corrected by introducing an extra term ‘exchange’
for the requirement of Pauli’s exclusion principle for antisymmetric wave function.
Also to get the precise understanding of the dielectric function the correlation effects
also becomes necessary to be introduced.

So, total potential energy is written as,

\[ V(q) = V_b(q) + V_s(q) + V_{ex}(q) \] (2.13)

Where, \( V_b(q) \) is bare ion-electron potential. \( V_s(q) \) is potential energy due to screening
effect and \( V_{ex}(q) \) is potential energy due to exchange and correlation effects.

In order to calculate the static screening effects we can use Thomas- Fermi
approach and we can write [2.13],

\[ \varepsilon(q) = \frac{V_b(q)}{\varepsilon(q)} \] (2.14)

where, \( K_{TF} \) is Thomas Fermi wave vector. For free electrons it is given by,

\[ V_s(q) = \frac{V_b(q)}{\varepsilon(q)} \] (2.15)

In terms of self consistent scheme the screening term \( V_s(q) \) can be written as [2.12],

\[ V_s(q) = \frac{4\pi e^2 X_q}{q^2} \] (2.16)

Using perturbation theory we can find out,

\[ X_q = \frac{q^2 V(q)}{4\pi e^2} \left[ 1 + \varepsilon_H(q) \right] \] (2.17)
Where, \( \varepsilon_H(q) \) is static Hartree dielectric function given by [2.13],
\[
\varepsilon_H(q) = 1 + \frac{me^2}{2\pi k_F \hbar (q / 2k_F)^2} \left[ \frac{1 - (q / 2k_F)^2}{2(q / 2k_F)} \right] \ln \left[ \frac{1 + (q / 2k_F)}{1 - (q / 2k_F)} \right]
\]  
(2.18)

We can find out by substitution,
\[
V_s(q) = V(q)[1 - \varepsilon_H(q)]
\]  
(2.19)

And hence,
\[
V(q) = V_b(q) + V_s(q)
\]

\[
\therefore V(q) = V_b(q) + V(q)[1 - \varepsilon_H(q)]
\]

\[
\therefore V_b(q) = V(q)[1 - (1 - \varepsilon_H(q))]
\]

\[
\therefore V(q) = V_b(q) / \varepsilon_H(q)
\]  
(2.20)

Here, exchange and correlation effects have not taken into account.

The exchange and correlation effects among conduction electrons are required by Pauli’s exclusion principle. It can be found from many body perturbation theories. Correlation effects arise from the columbic repulsion between the electrons. Such repulsion gives rise to correlation hole around each electron. In order to involve the exchange and correlation effects, we can use term \( v_s \) which represent average interaction between electrons [2.13].
\[
V_{ex}(q) = a_s \chi_q
\]  
(2.21)

Using equation 2.16, we can write,
\[ V_s(q) + V_m(q) = \left( \frac{4\pi e^2}{q^2} \right) \chi_q + a_v \chi_q \]

\[ = \left( \frac{4\pi e^2}{q^2} \right) \left[ 1 - f(q) \right] \chi_q \]

where, \( f(q) = \frac{q^2}{4\pi e^2} a_v \)

Finally, we get by substitution,

\[ V(q) = \frac{V_b(q)}{1 + \left[ (\varepsilon(q) - 1) \cdot (1 - f(q)) \right]} \]

\[ \therefore V(q) = V_b(q) / \varepsilon(q) \]

Where, \( \varepsilon(q) = 1 + \left[ (\varepsilon_H(q) - 1) \cdot (1 - f(q)) \right] \)

Thus we can find out the form of screened pseudopotential.

There are many forms of possible local field correction functions which are proposed to incorporate the exchange and correlation effects among conduction electrons. In the present investigation, we have used six different form of local field correction functions viz. Hartree function (H) [2.2], Taylor function (T) [2.14], Hubbard and Sham (HS) [2.15, 2.16], Ichimaru-Utsumi function (IU) [2.17], Farid et al. function (F) [2.18] and Sarkar et al. function (S) [2.19].

### 2.3.1 Local field correction function

#### 1. Hartree (H) function

As the H dielectric is purely be static one and does not include exchange and correlation effects, the local-field correction becomes

\[ f(q) = 0.0 \]
2. Taylor (T) function

Taylor [2.14] has suggested a very simple expression for \( f(q) \), which satisfies the compressibility sum rule and, in general, covers the overall feature of local-field correction function proposed before 1972. According to Taylor [2.14]

\[
f(q) = \frac{q^2}{4K_F^2} \left[ 1 + \frac{0.1534}{\pi K_F^2} \right]
\]  

(2.28)

3. Hubbard and Sham (HS) local field correction function

Hubbard and Sham (HS) [2.15, 2.16] proposed a simple form of local –field correction function, which is of the form

\[
f(q) = \frac{q^2}{2(q^2 + \xi_1 K_F^2)} , \quad \text{where, } \xi_1 = \frac{0.916}{[0.458 + (0.012 \cdot r_s)]}
\]  

(2.29)

Where, \( r_s \) is define the wiegner-Size radius.

4. Ichimaru and Utsumi (IU) Local field Correction function

The local field function of IU [2.11] is fitting formula for the dielectric screening function of the degenerate electron liquids at metallic and lower densities, which accurately reproduces the Monte-Carlo results as well as those of the microscopic correlations and which satisfies the self-consistency condition in the compressibility sum rule and short range correction. The mathematical formula is

\[
f(q) = AQ^4 + BQ + C + \left[ AQ^4 + \left( B + \frac{3A}{8} \right) Q^2 - C \right] \left[ \frac{4Q^2}{Q^2} \ln \frac{2+Q}{2-Q} \right]
\]  

(2.30)

Where, \( A, B, C \) are the \( r_s \) dependent parameter and \( Q=q/k_F \)

\( A=0.029 \quad (0 \leq r_s \leq) \)
\[ B = \left( \frac{9}{16} \right) \cdot \gamma_0 - \left( \frac{3}{64} \right) \cdot (1 - g(0)) - \left( \frac{16}{15} \right) \cdot A \]

\[ C = \left( -\frac{3}{4} \right) \cdot \gamma_0 + \left( \frac{9}{16} \right) \cdot (1 - g(0)) - \left( \frac{16}{15} \right) \cdot A \]

Where,

\[ \gamma_0 = 0.25 - \left( \frac{\pi}{24} \right) \cdot \left( \frac{4}{9\pi} \right)^{\frac{1}{2}} \cdot r_s^5 \cdot \frac{d}{dr_s} \left( r_s^{-2} \cdot \frac{d}{dr_s} E_c(r_s) \right) \]

and \( g(0) = \frac{1}{8} \int \frac{Z}{I_1(Z)} \]

Here \( I_1(Z) \) is the first order modified Bessel’s function and \( E_c(r_s) \) is the correlation energy.

5. Farid et al (F) local field correction function

On the basis of IU [2.17] function, Farid et al. (f) [2.18] have given a local field correction that is of the form

\[ f(q) = AQ^4 + BQ^2 + C + \left[ AQ^4 + DQ^2 - C \right] \frac{4 - Q^2}{4Q} \ln \left| \frac{2 + Q}{2 - Q} \right| \] (2.31)

With \( Q = q/k_F \) and A, B, C and D are the \( r_s \) dependent parameter. This function also satisfied the compressibility sum rule.

\[ A = \frac{63}{64} a_0 + \frac{15}{4096} (b_0^4 - 2(b_0^a + b_0^c)) - 16b_{-2} \]

\[ B = \frac{9}{16} \gamma_0 + \frac{7}{16} b_{-2} - \frac{3}{64} b_0 - \frac{16}{15} A \]

\[ C = -\frac{3}{4} \gamma_0 + \frac{3}{4} b_{-2} - \frac{9}{16} b_0 - \frac{16}{5} A \]

\[ D = \frac{9}{16} \gamma_0 - \frac{9}{16} b_{-2} - \frac{3}{64} b_0 + \frac{8}{5} A \]

Where, constant \( b_0^4, b_0^a, b_0^c, b_{-2} \) and \( \gamma_0 \) are well defined in Farid et al. [2.18]. The parameter A, B, C and D appearing in the expression are well defined in the respective article [2.18].
6. Sarkar et al (S) local field correction function

Sarkar et al. (S) proposed a simple form of local field correction function, which is of the form

\[ f(q) = A \left[ 1 - \left\{ 1 + BQ^4 \right\} \exp(-CQ^4) \right] \quad (2.32) \]

Here, A, B and C are \( r_s \) dependent parameter. This function satisfied the compressibility sum rule.

where, \( B = a + br_s + cr_s \log r_s + (d \log r_s) r^2_s + \left( e/r_s^3 \right) \)

with

\[ a = 0.0301412 \]
\[ b = -0.0084724176 \]
\[ c = 0.0016291083 \]
\[ d = -0.2386599 \]
\[ e = 0.027960609 \]

Here, constant \( A \) and \( C \) are determine from the limit values of \( f(q) \)

\[ \lim_{q \to \infty} f(q) = 1 - g(0) \]

where,

\[ g(0) = \frac{1}{8} \left[ \frac{Z}{I_1(Z)} \right]^2 \]

The constant \( C \) can be found using,

\[ \lim_{q \to 0} f(q) = AC \left( q/k_F \right) \]

\[ \therefore \gamma_0 = AC \]

\[ \therefore C = \frac{\gamma_0}{1 - g(0)} \]

\( \gamma_0 = 0.25 - \left( \frac{\pi}{24} \right) \left( \frac{4}{9\pi} \right)^\frac{1}{2} \int r_s^5 \frac{d}{dr_s} \left( r_s^{-2} \frac{d}{dr_s} E_c(r_s) \right) \)
In expression [2.14-2.19], $Q = q/k_F$. The nature of these $f(q)$s are plotted in figure 2.1 and the dielectric function $\varepsilon(q)$s are shown in figure 2.2. These curves are drawn for aluminium for sake of comparison only.

It is seen from figure 2.1 that local field correction due to IU and F showing peak at around $q=2k_F$. These $f(q)$s are involving the logarithmic singularity at $q=2k_F$. all these functions approaches to zero as $q \to 0$. At $q \to \infty$ the limiting behaviour of these functions is given as:

\[
\begin{align*}
    f(q) & \to \infty & \text{For T and F} \\
    f(q) & \to 1-g(0) & \text{For IU} \\
    \text{and } f(q) & \to C & \text{For S}
\end{align*}
\]

Figure 2.2: Different local field correction functions for the Aluminium.
From the figure 2.2, it is observed that inclusion of various local field correction to the dielectric functions $\varepsilon(q)$, suppresses the static Hartree (H) dielectric function in the entire range of wave vector $q$.

Figure 2.3: Modified dielectric functions for Aluminium.
2.4 Model Potentials

The pseudopotential theory, in the different forms has done tremendous job in giving the understanding of large number of metallic properties of simple metals since the last five decades [2.20-2.54]. However, the applicability of local model pseudopotential to metals, binary complexes and bulk metallic glasses is long standing problem and it still remains a problem of interest in the field of condensed matter theory, materials science and engineering. During last five decades, various physical properties of liquid metals, liquid semiconductors and alloys as well as glasses composed of metals are studied [2.20-2.54]. But it is found that most of these studies are scattered in the sense that given pseudopotentials have not been consistently exploited for the comprehensive studies of structural related properties, electrical transport properties, dynamic, atomic properties. In the scattered studies, different author have used different phenomenology and hence different forms in real-space with relevant parameters determined differently. The local-field correction functions in the dielectric function have also been used with different approximations.

Looking at the above factors and the literature survey made for the Ph.D. thesis, we are motivated by the work of Jani et al. [2.40-2.50]. Therefore we have selected two different types of model potentials one in r-space (exponential) pseudopotential and a second one is in q-space (empirical), to study comprehensively metals binary alloys and some bulk metallic glasses while incorporating six different local field correction functions. In the present thesis these models have explained various properties of metallic complexes, comprehensively. The first model potentials used in the present work is given r-space (Model-1) [2.43, 2.44] as:

\[
V_{\text{ion}} = -\frac{Ze^2}{r} \quad \text{for } r < r_c
= -\frac{Ze^2}{r} + \frac{Ze^2}{r_c} \exp\left(-\frac{r}{r_c}\right) \quad \text{for } r \geq r_c
\]  (2.33)

This form has feature of columbic terms outside the core and varying cancellation due to a repulsive and an attractive contribution to the potential within the core. It is assumed that the potential within the core should not be zero nor...
constant but it should vary as a function of \( r \). The Fourier transform of this pseudopotential in the Fermi wave vector space is written as

\[
V_s(q) = -\frac{4\pi Z e^2}{\Omega_0 q^2 \varepsilon(q)} \left[ \cos(q r_c) \cdot \frac{\exp(-1)q r_c}{(1 + q^2 r_c^2)} \{\sin(q r_c) + q r_c \cos(q r_c)\} \right]
\]  

(2.34)

This is a single parametric local model potential whose parameter \( r_c \) is found from the values of the wave vector \( q_0 \), where the form factor takes first zero value. For the present model the condition yields,

\[
r_c = \frac{1.34392}{\left[ q_0 \left( \frac{2}{k_F} \right)^2 \right]}. \quad (2.35)
\]

Another pseudopotential used in the present work is proposed by Gajjar and Jani et al. [2.43, 2.52] directly in q-space (Model-2) which is of the form,

\[
V_s(q) = -\frac{4\pi Z e^2}{\Omega_0 q^2 \varepsilon(q)} \left[ \cos(q R_c) - \frac{q^2 r_c^2}{(1 + q^2 r_c^2)} \right]
\]  

(2.36)

This model potential is the modified version of the well known Ashcroft model in reciprocal space. Gajjar & Jani has introduced second term for making the model weaker.

\[
r_c = \frac{1.03003}{\left[ q_0 \left( \frac{2}{k_F} \right)^2 \right]}. \quad (2.37)
\]

Here \( Z, \Omega_0, q, r_c \) and \( \varepsilon(q) \) are the valency, atomic volume, wave vector, the potential parameter and dielectric function, respectively.
In the present investigation the parameter, $r_c$ is calculated from $q=q_0$ value. In the case of non availability of experimental $q_0$ value, $r_c = 0.51 \frac{R_a}{Z} Z^{-1/3}$ relation is used [2.3, 2.54]. Where $R_a$ atomic radius and $Z$ is the valency of the given metal.

For the investigation of various properties of $A_{1-x}B_x$ binaries, the input parameters and constants needed are determined using following relations.

$$Z = Z_A(1-x) + Z_Bx$$
$$\Omega_0 = \Omega_{0A}(1-x) + \Omega_{0B}x$$
$$k_F = k_{FA}(1-x) + k_{FB}x$$
$$M = M_A(1-x) + M_Bx$$

The calculated parameter $r_c$ and other constant, for the some alkaline earth metals and transition metals used in the present investigation are tabulated in Table 2.1.

<table>
<thead>
<tr>
<th>Metals</th>
<th>z</th>
<th>$M$ (a.m.u)</th>
<th>$k_F$ (a.u)</th>
<th>$\Omega_0$ (a.u)</th>
<th>$r_s$ (a.u)</th>
<th>$r_c$ (a.u) Model-1</th>
<th>$r_c$ (a.u) Model-2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Al</td>
<td>3</td>
<td>26.98</td>
<td>0.88642</td>
<td>127.533</td>
<td>2.16507</td>
<td>0.9974</td>
<td>0.7645</td>
</tr>
<tr>
<td>Ca</td>
<td>2</td>
<td>40.08</td>
<td>0.56536</td>
<td>327.710</td>
<td>3.39462</td>
<td>1.4150</td>
<td>1.0845</td>
</tr>
<tr>
<td>Cr</td>
<td>1</td>
<td>52.00</td>
<td>0.68308</td>
<td>92.898</td>
<td>2.80957</td>
<td>1.4329</td>
<td>1.4329</td>
</tr>
<tr>
<td>Co</td>
<td>1</td>
<td>58.93</td>
<td>0.70159</td>
<td>85.738</td>
<td>2.73545</td>
<td>1.3951</td>
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<tr>
<td>Ni</td>
<td>1</td>
<td>58.71</td>
<td>0.70315</td>
<td>85.163</td>
<td>2.72937</td>
<td>1.3920</td>
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<td>0.69209</td>
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<td>Sr</td>
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<td>0.52365</td>
<td>412.411</td>
<td>3.66497</td>
<td>1.5277</td>
<td>1.1712</td>
</tr>
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<td>0.85141</td>
<td>191.892</td>
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<td>121.75</td>
<td>0.82557</td>
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<td>2.32465</td>
<td>0.9926</td>
<td>0.7608</td>
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<td>Ba</td>
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<td>463.365</td>
<td>3.81009</td>
<td>1.5512</td>
<td>1.1889</td>
</tr>
</tbody>
</table>

After evaluation of the parameter of the potential the computation of the form factor becomes straightforward. Figure 2.3 shows the real space nature of the potential while figure 2.4 shows the screened form factors in $q$-space for different concentration of the metallic glasses. In the figure 2.2 form factors due to the Taylor [2.52] dielectric screening function are shown to avoid complications.
Figure 2.4: Model Potential (in r-space) for given metals
Figure 2.5: Form factor for given metals using Model-1 & Model-2 potential
First we discuss the features of real space version shown in Figure: 2.4

- It seen that when we move from valency \( Z=1 \) to \( Z=4 \) the size of the Pseudo–core increases while the depth of the potential within the core increases.
- The lowest \( r_c \) is obtained for Sr metals while the highest \( r_c \) is obtained for Ba.
- This gives the relation between the atomic volume and the minimum of the potential or the potential at \( r_c \). The relation is of the type.

\[
V(r=r_c) = a_0 + a_1 \Omega_0 + a_2 \Omega_0^2 + a_3 \Omega_0^2
\]

Following points are noted from Figure: 2.5

- The form factors generate correct limiting values \( V_S(q) \rightarrow (-2/3)E_F \) as \( q \rightarrow 0 \) and \( V(q)\rightarrow0 \) as \( q\rightarrow\infty \).
- Form factors give stable and almost consistent behaviour in the physically important region of wave vector \( q \).
- The form factors are free from any abnormal and unwanted oscillation.
- Proper convergence arises for higher wave vector \( q \).

The above generated form factors are then used to study structure related properties, Electrical transport properties, phonon dispersion relations, velocity auto correlation functions, total energy, pressure volume relation and Fermi surface distortion.
CHAPTER 2

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