

Calculation of short range order in Ni–Rh, Ni–Pd and Cu–Rh alloys

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Transition metal model pseudopotential (TMMP) technique has been applied to study the short range order (SRO) in nickel alloys $\text{Ni}_{100-x}\text{-Rh}_x$ and $\text{Ni}_{100-x}\text{-Pd}_x$ and a copper alloy $\text{Cu}_{100-x}\text{-Rh}_x$ ($x = 2, 5, 8, 11$ at. %). All these transition metal alloys form *fcc* solid solutions for the chosen compositions. The static electrical permittivity $\epsilon(q)$ was taken from the Hubbard–Sham model and/or Geldart–Vosko model to account for the exchange energies and correlation correction factors. Ordering energies and the Warren–Cowley SRO parameters have been calculated for all these alloys. Both models gave almost the same values for both the ordering energies and the Warren–Cowley SRO parameters. The TMMP model is found to predict the correct sign of SRO parameters for all these alloys.

Key words: *clustering; lattice constant; pseudopotential theory; transition metal model pseudopotential*

1. Introduction

Short range order (SRO) is an arrangement of atoms in the immediate neighbourhood of a particular atom in the lattice. It can decrease with increasing distance and can be restricted to the microcrystals which are joined to one another in a disjointed fashion. SRO is thus related to those arrangements where unlike atoms tend to become near neighbours [1]. Tendency for like atoms to be near neighbours is named as clustering. SRO, its degree, type and sign depend on concentration, nature, temperature of solid solution and history of the specimen [2]. The degree of SRO could be related to the diffraction effects produced. In terms of a suitable parameter termed as the Warren–Cowley parameter α_i (WCP) SRO can be defined as [1]:

$$\alpha_i = 1 - \frac{P_A^i}{C_A} = 1 - \frac{P_B^i}{C_B}$$

where P_A^i, P_B^i denote the conditional probabilities of having B and A atoms as neighbours in the i -th coordination sphere, respectively, and C_A and C_B are concentra-

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tions of atoms A and B. Being composed of like and unlike atoms with particular forces of attraction or repulsion operating between them, all real solid solutions probably exhibit either short range order or clusters to a greater and lesser degree [3]. The presence of SRO may be decided based on the value of the Warren–Cowley parameter α_i :

- $\alpha_i < 0$ for SRO,
- $\alpha_i > 0$ for clustering or local order,
- $\alpha_i = 0$ for complete randomness.

Differences in the interatomic pair interaction energies E_{AB} of the AA, BB and AB pairs in an i -th coordination sphere, defined by $E_{AB} = V_{AB} - 1/2(V_{AA} + V_{BB})$, may cause SRO formation [1]. Ordering energy determines the tendency of atoms to order in the system, e.g. an increase in the number of AB pairs ($E_{AB} > 0$), i.e. SRO formation or decrease in the number of AB pairs ($E_{AB} < 0$), i.e. disordering. The absolute value of the ordering energy near the critical temperature T_C is $E_{AB} = k_B T_C$ below which lies the long range order (LRO) and above which lies SRO, which becomes weaker with the increase of temperature leading to a random statistical distribution of atoms at high temperatures.

In solid solution alloys, SRO is usually described by two basic models: homogeneous and heterogeneous ones. The homogeneous model assumes that ordering proceeds uniformly throughout the specimen, i.e. for any site i occupied by A atom, there will be some probability (independent of the choice of i) that adjacent sites will be occupied by atoms of different kind (B). As there is no correlation between distinct sites, widely separated regions may or may not contain the same ordering sequence. On the other hand, the heterogeneous model involves the development of SRO by the emergence of small domains (which may differ in composition from that of the nominal alloy) having some equilibrium degree of order (micro-domain model). These domains have dimensions lower than the coherence length (i.e., electron mean free path). The anti-phase domain model assumes that early stages of ordering are characterized by a very fine random network of anti-phase domains, each domain having some equilibrium degree of order. In both micro-domain and anti-phase domain models, if the domain size is lower than the coherence length, such ordering will result in diffuse scattering and be properly classified as SRO.

High resolution electron microscopy (HREM) can be used to gain information about the type of SRO prevailing in a system or SRO can be indirectly studied by a detailed analysis of the diffuse scattered intensity with the assistance of some of the modeling techniques. Valuable additional information can also be obtained by using probes of different coherence lengths (e.g., Mössbauer effect, neutron scattering and resistivity). X-ray and neutron diffraction techniques have been used to study SRO mainly due to the reason that they provide a direct measurement of the degree of SRO. The SRO parameters have been determined experimentally for a large number of metallic solid solutions by diffuse X-ray/neutron scattering intensity measurements (DSIM) [4–12]. Vrijen and Radelaar [13] observed in Cu–Ni alloys that cluster parameters had a strong asymmetry in their composition dependence. Electrical resistivity measurements were used to study SRO in various metallic systems [10, 12, 14].

The differential scanning calorimetry (DSC) was applied for SRO studies in mechanically alloyed $\text{Hf}_{7.5}\text{Al}_{7.5}\text{Cu}_{7.5}\text{Ni}_{10}$ and amorphous $\text{Zr}_{7.5}\text{Al}_{7.5}\text{Cu}_{7.5}\text{Ni}_{10}$ alloys [15]. Bliznuk et al. [16] studied the effect of nitrogen on SRO in duplex steel by Mössbauer spectroscopy, internal friction and the Cowley parameters measurements. Theoretical investigations of SRO have been made by various simulation techniques using statistical and electronic theories of SRO as well as pseudopotential theory. Gruner et al. [9] and Kramer and Sordelet [17] applied reverse Monte Carlo simulation technique to study SRO and atomic clusters in Cu–Sn and Zr–Pd alloys, respectively. Electronic theory of ordering has been applied to calculate SRO parameters in Ni–Rh and Ni–Ir alloys by Abbas et al. [5]. The SRO investigations have also been performed using the pseudopotential theory for the calculations of many atomic properties and was found useful for studying ordering characteristics of alloy formation, if not for all, then at least for a series of groups [4, 18]. Khawaja et al. [19] and Abbas et al. [20, 21] used pseudopotential technique in the second order perturbation theory to calculate local ordering energy and showed good agreement with the experimental results.

In the present investigations, the transition metal model pseudopotential (TMMP) technique has been successfully applied to study the SRO in Ni–Rh, Ni–Pd and Cu–Rh alloys in the second order perturbation theory. The Warren–Cowley SRO parameters, as modified by Katsnelson et al. [22], and local ordering energies have been calculated using the dielectric screening function $\varepsilon(q)$ in the Hartree approximation [23], and the energy exchange and correlation correction parameters $f(q)$ by applying two different approaches as proposed by Hubbard and Sham [24, 25], and Geldart and Vosko [26]. This research is the continuation of our earlier work on SRO [20, 21].

2. Theory of ordering energy and the Warren–Cowley SRO parameters

According to the second order perturbation theory, the band structure contribution to the structure and configuration dependent part of the total energy [19] may be defined as:

$$E_{bs} = \frac{\Omega_0}{8\pi} \sum_q q^2 F'(q) \quad (1)$$

where $\Omega_0 = \Omega/N$ is the volume per atom and N is the number of atoms in a crystal of volume Ω . $F'(q)$ denotes the energy wave number characteristics. In the local pseudopotential approximation [27], $F'(q)$ may be expressed as:

$$F'(q) = |W^0(q)|^2 \frac{\varepsilon(q) - 1}{\varepsilon^*(q)} \quad (2)$$

here $W^0(q)$ is the local approximation of total unscreened pseudopotential form factor and is related to the wave number q :

$$W^0(q) = -\frac{4\pi z e^2}{\Omega_o} \cos\left(\frac{qR_m}{q^2}\right) \quad (2a)$$

whereas $\varepsilon(q)$ is the static electrical permittivity. In the Hartree approximation [22], it is given by:

$$\varepsilon(q) - 1 = \left(\frac{4\pi z e^2}{\Omega_o q^2}\right) \chi\left(\frac{q}{2K_F}\right) \quad (2b)$$

and $\varepsilon^*(q)$ is the modified dielectric screening function which accounts for the exchange and correlation effect and is defined as:

$$\varepsilon^*(q) = 1 + [1 - f(q)] [\varepsilon(q) - 1] \quad (3)$$

The term $\chi(q)$ represents the perturbation characteristic expressed by:

$$\chi(q) = \frac{3E_F^{-1}}{2} \left[\frac{1}{2} + \frac{4K_F^2 - q^2}{8K_F q} \ln \left| \frac{2K_F + q}{2K_F - q} \right| \right] \quad (4)$$

here $E_F = \frac{\hbar^2 K_F^2}{2m}$ is the Fermi energy,

$$K_F = \left(\frac{3\pi^2 Z}{\Omega} \right)^{1/3}$$

the Fermi vector and $f(q)$ is the exchange and correlation correction factor. According to Hubbard-Sham [24, 25] and Geldart-Vosko [26], $f(q)$ can be expressed as follows:

• Hubbard–Sham:

$$f(q) = \frac{q^2}{2} [q^2 + K_F^2 + K_S^2]^{-1} \quad (5)$$

where K_S is a screening parameter and can be written in terms of K_F as:

$$K_S^2 = \frac{2K_F}{\pi} \quad (5a)$$

• Geldart–Vosko:

$$f(q) = \frac{q^2}{2} [q^2 + \xi K_F^2]^{-1} \quad (6)$$

where $\xi = 2(1 + 0.026(m^*/m)\gamma_s)$ and $\gamma_s < 2$, γ_s is taken as unity, m is the mass of electron and m^* is its effective mass.

The SRO-dependent part of the band structure energy [19] may be written as:

$$E_{bs}^{\text{SRO}} = \frac{\Omega_0}{8\pi} \frac{c(1-c)}{N} \sum_R \sum_q q^2 \alpha(R) e^{iqR} \left| \Delta W^0(q) \right|^2 \frac{\varepsilon(q) - 1}{\varepsilon^*(q)} \quad (7)$$

Similarly, the SRO-dependent part of the electrostatic energy contribution to the total energy of the crystal may be given in the form:

$$E_{es}^{\text{SRO}} = \frac{c(1-c)}{N} \sum_q \sum_R \frac{(Z_A - Z_B)^2}{2} \frac{4\pi}{\Omega_0 q^2} e^{(-q^2/4\eta)} \alpha(R) e^{iqR} \quad (8)$$

where Z_A , Z_B are valences of the component atoms A and B of the A–B alloy, and η is the Ewald parameter defined as $\eta = \alpha_{\text{eff}}/\Omega^{1/3}$. By adding Eqs. (7) and (8), the expression for the total energy of the crystal [19] may be written as:

$$E^{\text{SRO}} = E_{bs}^{\text{SRO}} + E_{es}^{\text{SRO}} = \frac{c(1-c)}{N} \sum_q \sum_{\{R\}} \alpha(R) e^{iqR} F(q) \quad (9)$$

where $F(q)$ is an additive energy wave number characteristics depending upon the band structure and electrostatic energy contributions:

$$F(q) = \frac{\Omega_0}{8\pi} q^2 \left| \Delta W^0(q) \right|^2 \frac{\varepsilon(q) - 1}{\varepsilon^*(q)} + 2\pi \frac{(Z_A - Z_B)^2}{\Omega_0 q^2} e^{(-q^2/4\eta)} \quad (10)$$

Changing the summation in Eq. (9) to integration and averaging it over all lattice sites q and R , the total energy of the crystal can be rewritten as:

$$E^{\text{SRO}} = c(1-c) \sum_{\{R_i\}} \alpha(R_i) e^{iqR} V(R_i) \quad (11)$$

where

$$V(R_i) = \frac{\Omega_0}{\pi^2} \int dq q^2 F(q) \frac{\sin(qR_i)}{qR_i} \quad (12)$$

$V(R_i)$ being the local ordering energy of the i -th coordination sphere of the radius R_i [28].

Using the expression for the entropy [21], the Warren–Cowley SRO parameter α_1 for the first coordination sphere can be written as:

$$\frac{\alpha_1}{(1 - \alpha_1)^2} = c(1 - c) \left[e^{-V(R_1)/(k_B T)} - 1 \right] \quad (13)$$

where k_B is the Boltzmann constant.

3. Results and discussion

Transition metal model pseudopotential (TMMP) technique has been applied to study the short range order (SRO) in two nickel alloys: Ni–Rh and Ni–Pd, and in a copper alloy Cu–Rh. All these transition metal alloys form *fcc* solid solutions for the chosen compositions. The static electrical permittivity $\epsilon(q)$ in this study is either from Hubbard–Sham [24, 25] or from Geldart–Vosko [26].

3.1. Ni–Rh system

The phase diagram of Ni–Rh system has not been completely established [29] but it appears that the solid Ni lattice can accommodate large amount of Rh before the solubility limit is exceeded. The lattice constants for the *fcc* Ni–Rh alloys have been calculated based on an average lattice and are given in Table 1. It is clear from this table that the lattice parameter a increases with increasing Rh content. This rise of a could be associated with the size of two elements. The radii of coordination spheres are related to the lattice constants. The calculated radii of the first three coordination spheres are also presented in the same table, which also show a slight rise with increasing Rh concentration in the Ni–Rh alloys.

Table 1. Lattice constants and radii of coordination spheres in Ni–Rh alloys

Rh content [at. %]	$R_1 = \frac{a}{\sqrt{2}}$ [Å]	$R_2 = a$ [Å]	$R_3 = \sqrt{2}a$ [Å]
2	2.4929	3.5256	4.9859
5	2.4998	3.5340	4.9978
8	2.5048	3.5424	5.0097
11	2.5048	3.5424	5.0097

$$a_{\text{Ni}} = 3.52 \text{ \AA}, a_{\text{Rh}} = 3.84 \text{ \AA}$$

Ordering energies $V(R_i)$ of three coordination spheres and the short range order parameters α_i were calculated by applying Eqs. (12) and (13) using a computer program written in MATLAB 7. The input parameters for TMMP calculations for Ni–Rh alloys, taken from Animalu [30], are given in Table 2.

Table 2. Input parameters for the transition metal model pseudopotential used in the calculation of ordering energy $V(R_i)$

Metal	R_m	Ω	Z	$ R_c $	α_{eff}	E_C	η
Ni	2.2	73.6	2	1.304	0.063	0.093	0.0150
Pd	2.6	99.3	2	1.512	0.073	0.091	0.0157
Rh	2.0	92.6	3	1.258	0.048	0.960	0.0106
Cu	2.2	79.4	1	1.814	0.157	0.960	0.0365

The ordering energies thus calculated for three coordination spheres are given in Table 3.

Table 3. Ordering energies for Ni–Rh alloys calculated by taking into account the exchange and correlation correction parameters $f(q)$

Rh content [at. %]	$V(R_1)$ [a.u.]	$V(R_2)$ [a.u.]	$V(R_3)$ [a.u.]
Hubbard–Sham [24, 25]			
2	0.0005	–0.0008	–0.0005
5	0.0015	–0.0020	–0.0013
8	0.0023	–0.0031	–0.0020
11	0.0032	–0.0041	–0.0027
Geldart–Vosko [26]			
2	0.0005	–0.0008	–0.0005
5	0.0015	–0.0020	–0.0013
8	0.0023	–0.0031	–0.0020
11	0.0032	–0.0041	–0.0027

The table shows that ordering energies for the first coordination sphere are positive for all concentrations of Ni–Rh alloys but have negative values for the second and third coordination spheres. The values of ordering energies increase upon increasing Rh concentration. These results show that there is a tendency of unlike atoms (i.e., Ni–Rh) to be the nearest neighbours which indicates the short range order for the first coordination sphere but for the second and third ones, the probability of like atoms (i.e., Ni–Ni and Rh–Rh) is more likely indicating clustering.

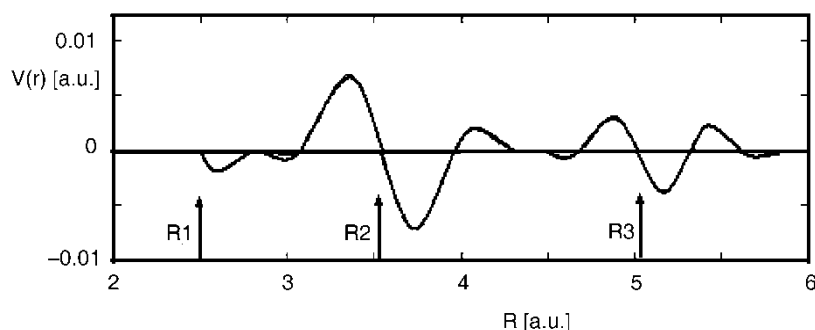


Fig. 1. Ordering energies $V(R)$ as a function of radii R of the coordination spheres in $\text{Ni}_{89}\text{Rh}_{11}$ alloys

This behaviour shows semi-oscillatory characteristics of ordering energies (Fig. 1). This result is also obvious from the Warren–Cowley SRO parameters as presented in Table 4, where negative values of α_1 refer to short-range order but positive

values of α_2 and α_3 refer to clustering [20]. The present results are found to be in good agreement with those of Abbas [5].

Table 4. Warren–Cowley SRO α_i parameters for Ni–Rh alloys

Rh content [at. %]	α_1	α_2	α_3
Habbard–Sham [24, 25]			
2	–0.0004	0.0006	0.0004
5	–0.0011	0.0014	0.0009
8	–0.0017	0.0021	0.0014
11	–0.0024	0.0028	0.0019
Geldart–Vosko [26]			
2	–0.0004	0.0006	0.0004
5	–0.0011	0.0014	0.0009
8	–0.0017	0.0021	0.0014
11	–0.0024	0.0028	0.0019

3.2. Ni–Pd system

The phase diagram of Ni–Pd alloy shows that it crystallizes in a complete series of solid solution alloys [29]. The lattice constants for the *fcc* Ni–Pd alloys have been calculated based on an average lattice (Table 5). It is clear that the lattice parameter a increases with increasing Pd content. This rise of a could be associated with the size of two elements. The calculated radii of the first three coordination spheres are also presented in Table 5, which also show a slight increase with increasing Pd concentration in the Ni–Pd alloys.

Table 5. Lattice constants and radii of coordination spheres in Ni–Pd alloys

Pd content [at. %]	$R_1 = \frac{a}{\sqrt{2}}$ [Å]	$R_2 = a$ [Å]	$R_3 = \sqrt{2}a$ [Å]
2	2.4942	3.5274	4.9884
5	2.5020	3.5385	5.0041
8	2.5099	3.5496	5.0198
11	2.5177	3.5607	5.0355

$$a_{\text{Ni}} = 3.52 \text{ Å}, a_{\text{Pd}} = 3.89 \text{ Å}$$

Using MATLAB 7, the ordering energies $V(R_i)$ of three coordination spheres and the short range order parameters α_i have been calculated (Tables 6 and 7).

Table 6. Ordering energies for Ni–Pd alloys calculated by taking into account exchange and correlation correction parameters $f(q)$

Pd content [at. %]	$V(R_1)$ [a.u.]	$V(R_2)$ [a.u.]	$V(R_3)$ [a.u.]
Hubbard–Sham [24, 25]			
2	0.0002	–0.0008	–0.0001
5	0.0005	–0.0090	–0.0004
8	0.0009	–0.0012	–0.0007
11	0.0013	–0.0016	–0.0011
Geldart–Vosko [26]			
2	0.0002	–0.0008	–0.0001
5	0.0005	–0.0090	–0.0004
8	0.0009	–0.0012	–0.0007
11	0.0013	–0.0016	–0.0011

Table 7. Warren–Cowley SRO α_i parameters for Ni–Pd alloys

Pd content [at. %]	α_1	α_2	α_3
Hubbard–Sham [24, 25]			
2	–0.0002	0.0008	0.0001
5	–0.0004	0.0010	0.0004
8	–0.0007	0.0012	0.0007
11	–0.0009	0.0016	0.0011
Geldart–Vosko [26]			
2	–0.0002	0.0008	0.0001
5	–0.0004	0.0010	0.0004
8	–0.0007	0.0012	0.0007
11	–0.0009	0.0016	0.0011

Table 6 shows that ordering energies for the first coordination sphere are positive for all concentrations of Ni–Pd alloys but have negative values for the second and third coordination spheres, with a decreasing trend on increasing Pd concentration. These results show that there is a tendency of unlike atoms, i.e. Ni–Pd to be the nearest neighbours which indicate the short range order for the first coordination sphere but for the second and third coordination spheres the probability of like atoms, i.e. Ni–Ni and Pd–Pd is more likely indicating clustering. This behaviour points to a semi-oscillatory characteristic of ordering energies as is clear from Fig. 2. This result is also obvious from the Warren–Cowley SRO parameters as given in Table 7 where negative values of α_1 refer to short-range order but positive values of α_2 and α_3 refer to clustering [20, 21].

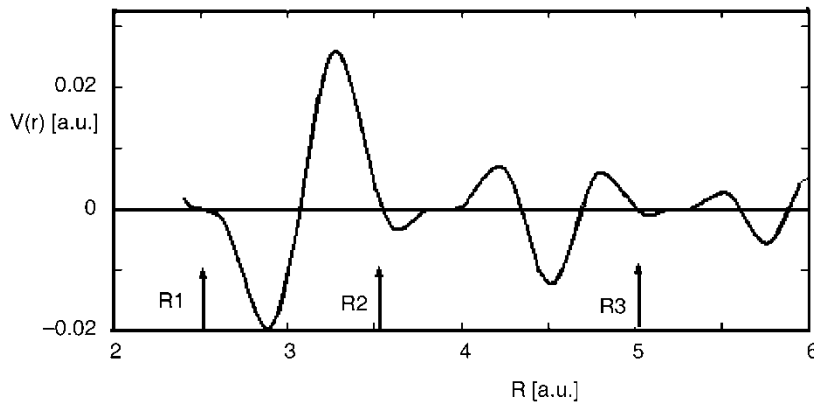


Fig. 2. Ordering energies $V(R)$ as a function of radii R of the coordination spheres in $\text{Ni}_{89}\text{Pd}_{11}$ alloy

3.3. Cu–Rh system

The Cu–Rh phase diagram [29] indicates a peritectic reaction at 1100 °C which suggests that a single phase exists in Cu–Rh alloys at 25 °C as primary solid solution of α -CuRh between 0 and 20 at. % Rh, and α -RhCu between 90 and 100 at. % Rh. The alloys of intermediate compositions are two-phase mixtures of α -CuRh and α -RhCu. Therefore, the chosen compositions of Cu–Rh alloys lie within that composition range (between 0 and 20 at. % Rh), which form α solid solutions. The lattice constants for the *fcc* Cu–Rh alloys calculated based on an average lattice using Vegard's rule are given in Table 8, which shows a rise in the lattice parameter a with increasing Rh content associated with its larger size as compared to Cu. The calculated radii of the first three coordination spheres are also presented in Table 8, which also show a slight rise with increasing Rh concentration in the Cu–Rh alloys.

Table 8. Lattice constants and radii of coordination spheres in Cu–Rh alloys

Rh content [at. %]	$R_1 = \frac{a}{\sqrt{2}}$ [Å]	$R_2 = a$ [Å]	$R_3 = \sqrt{2}a$ [Å]
2	2.5553	3.6238	5.1106
5	2.5593	3.6295	5.1187
8	2.5634	3.6252	5.1268
11	2.5674	3.6309	5.1348

$$a_{\text{Cu}} = 3.61 \text{ \AA}, a_{\text{Rh}} = 3.84 \text{ \AA}$$

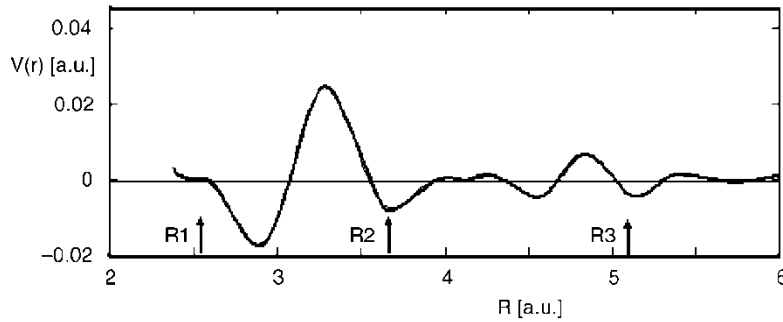
The calculated ordering energies for the three coordination spheres are presented in Table 9 and found positive for first coordination spheres for all concentration of Cu–Rh alloys but show negative values for second and third coordination spheres.

Table 9. Ordering energies for alloys Cu–Rh calculated by taking into account the exchange and correlation correction parameters $f(q)$

Rh content [at. %]	$V(R_1)$ [a.u.]	$V(R_2)$ [a.u.]	$V(R_3)$ [a.u.]
Hubbard–Sham [24, 25]			
2	0.0001	–0.0001	–0.0001
5	0.0003	–0.0003	–0.0002
8	0.0007	–0.0005	–0.0004
11	0.0008	–0.0007	–0.0005
Geldart–Vosko [26]			
2	0.0001	–0.0001	–0.0001
5	0.0003	–0.0003	–0.0002
8	0.0007	–0.0005	–0.0004
11	0.0008	–0.0007	–0.0005

Table 10. Warren–Cowley SRO α_i parameters for Cu–Rh alloys

Rh content [at. %]	α_1	α_2	α_3
Hubbard–Sham [24, 25]			
2	–0.0001	0.0001	0.0001
5	–0.0003	0.0002	0.0002
8	–0.0005	0.0004	0.0003
11	–0.0006	0.0005	0.0004
Geldart–Vosko [26]			
2	–0.0001	0.0001	0.0001
5	–0.0003	0.0002	0.0002
8	–0.0005	0.0004	0.0003
11	–0.0006	0.0005	0.0004

Fig. 3. Ordering energies $V(R)$ as a function of radii R of the coordination spheres in $\text{Cu}_{89}\text{Rh}_{11}$ alloy

The values of ordering energies increase with increase of Rh concentration. Therefore, the tendency of unlike atoms, i.e. Cu–Rh to be the nearest neighbours is high indicating SRO for the first coordination sphere and clustering seems to be more likely

due to the maximum probability of like atoms i.e. Cu-Cu and Rh-Rh to be nearest neighbours within the second and third coordination spheres. This result again represents a semi-oscillatory characteristic of ordering energies (Fig. 3). The SRO parameters (Table 10) also indicate a similar trend where negative values of α_1 refer to short-range order but positive values of α_2 and α_3 denote clustering [20, 21].

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