Static and Vibrational Properties of Equiatomic Rb-based Binary Alloys

Aditya M. Vora[1]
Humanities and Social Science Department, STBS College of Diploma Engineering,
Opp. Spinning Mill, Surat 395 006, Gujarat, India

The computations of the static and vibrational properties of four equiatomic Rb-based binary alloys viz. $Rb_{0.5}Li_{0.5}$, $Rb_{0.5}Na_{0.5}$, $Rb_{0.5}K_{0.5}$ and $Rb_{0.5}Cs_{0.5}$ to second order in local model potential is discussed in terms of real-space sum of Born von Karman central force constants for the first time. The local field correlation functions due to Hartree (H), Ichimaru-Utsumi (IU) and Sarkar et al. (S) are used to investigate influence of the screening effects on the aforesaid properties. Results for the lattice constants C_{11}, C_{12}, C_{44}, $C_{12}-C_{44}$, C_{12}/C_{44}, and bulk modulus B, obtained using the Hartree (H) local field correction function, have higher values in comparison to the results obtained for the same properties using Ichimaru-Utsumi (IU) and Sarkar et al. (S) local field correction functions. The results for the Shear modulus (C'), deviation from Cauchy's relation, Poisson's ratio σ, Young modulus Y, propagation velocity of elastic waves, phonon dispersion curves, and degree of anisotropy A are highly appreciable for the four equiatomic Rb-based binary alloys.

1. Introduction

In the study of various properties of solids, one frequently requires the knowledge of interaction energy between the ions or atoms. The studies of a pair effective interionic interaction in simple metals have a long history and originally they were not systematized and were concerned with individual groups of metals. In recent years considerable attention has been devoted to the theoretical study of the nature of effective interaction between the constituent atoms or ions in simple metals [1-4]. The bcc $A_{1-X}B_X$ (A=Rb; B=Li, Na, K, Cs) alloy system forms a substitutional solid solution in the overall region of concentration X of the second component and the crystal binding of the solid solution remains unchanged as compared to that of the pure alkali metals. Theoretical studies about the lattice dynamics of the alloy systems have been devoted to $Rb_{0.5}Li_{0.5}$, $Rb_{0.5}Na_{0.5}$, $Rb_{0.5}K_{0.5}$, and $Rb_{0.5}Cs_{0.5}$ systems since the lattice dynamics of the pure alkalis have been investigated in detail. But the work on the comprehensive study of static and vibrational properties of their binary alloys is almost negligible [1-9]. Only Soma et al. [7] have studied the phonon dispersion curves of $Cs_{0.7}K_{0.3}$, $Cs_{0.7}Rb_{0.3}$, $Cs_{0.3}Rb_{0.7}$ and $Rb_{0.71}Cs_{0.29}$ alloys. Vora and co-workers [1, 2] have reported the static and vibrational properties of equiatomic Na-based binary alloys using the model potential formalism. Very recently, Gajjar et al., have studied the lattice dynamics of bcc $Cs_{0.3}K_{0.7}$ alloy [3]. Experimentally, Kamitakahara and Copley [8] have studied the lattice dynamics of $Rb_{1-X}K_X$ alloys with X= 0.06, 0.18 and 0.29 by neutron scattering. Recently, Chushak and Baumketner [9] have reported the dynamical properties of liquid $Cs_{0.3}K_{0.7}$ alloy.

From a theoretical point of view, $A_{1-X}B_X$ (A=Rb; B=Li, Na, K, Cs) is a good system to study. Both constituents are members of an alkali metal group of the periodic table which, because of their relatively simple band structure, are generally the least complicated of all metallic systems to deal with. Assuming that a good description of both A and B metals can be utilized, a study of the alloy systems will shed a great deal of light on the general usefulness of the technique employed.

Hence, in the present article, we have decided to work for the first time on four equiatomic Rb-based binary alloys $Rb_{0.5}Li_{0.5}$, $Rb_{0.5}Na_{0.5}$, $Rb_{0.5}K_{0.5}$, and $Rb_{0.5}Cs_{0.5}$. Well-known single parametric local model potential of Gajjar et al. [1-3] is used to describe the electron-ion interaction. For the first time, an advanced and more recent, the local field correlation function method due to Ichimaru-Utsumi (IU) [10] and Sarkar et al. [11] has been employed in such investigations. This helps in identifying the influence of exchange and correlation effects in the static form of Hartree (H) (only static) dielectric function [12].

---

[1] voraam@yahoo.com

2. Theoretical Methodology

The phonon frequencies can be obtained by solving the standard secular determinental equation [1-5]

$$\det\left|D_{\alpha\beta}(q) - 4\pi^2\nu^2 M\,\delta_{\alpha\beta}\right| = 0 \qquad (1)$$

Where, M is the ionic mass, ν is the phonon frequency and $D_{\alpha\beta}(q)$ is the dynamical matrix in which the force between two ions depends only upon the distance between them is given by,

$$D_{\alpha\beta}(q) = \sum_n \left(1 - e^{i\mathbf{qr}}\right) \left.\frac{d^2\Phi(r)}{dr_\alpha\, dr_\beta}\right|_{r=r_n} \qquad (2)$$

Here, $\Phi(r)$ is the inter-ionic pair potential, r_α and r_β are α^{th} and β^{th} Cartesian components of the position vector of n^{th} ion, respectively.

This dynamical matrix element used in the present calculation finally takes the form,

$$D_{\alpha\beta}(q) = \sum_n \left(1 - e^{i\mathbf{qr}}\right)\left[K_t + \frac{r_\alpha r_\beta}{r^2}\left(K_r - K_t\right)\right] \qquad (3)$$

Here K_t and K_r are the force constants between a pair of ions interacting through a central interaction and n specifies shell index.

$$\begin{aligned} K_t &= \frac{1}{r}\frac{d\Phi(r)}{dr} \\ &= -\frac{Z^2e^2}{r^3} + \frac{\Omega_0}{\pi^2 r^2}\int_0^\infty F(q)q^2 \\ &\qquad \left[\cos(qr) - \frac{\sin(qr)}{q\,r}\right]dq \end{aligned} \qquad (4)$$

$$\begin{aligned} K_r &= \frac{d^2\Phi}{dr^2} \\ &= \frac{2Ze^2}{r^3} + \frac{\Omega_0}{\pi^2 r^2}\int_0^\infty F(q)q^2 \\ &\qquad \left[\frac{2\sin(qr)}{qr} - 2\cos(qr) - qr\sin(qr)dq\right] \end{aligned} \qquad (5)$$

Where, $F(q)$ is the energy wave number characteristic given by

$$F(q) = \frac{\Omega_0 q^2}{8\pi e^2}\left|W_B(q)\right|^2 \frac{\left[\varepsilon_H(q) - 1\right]}{1 + \left[\varepsilon_H(q) - 1\right]\left[1 - f(q)\right]} \qquad (6)$$

Here, $\Omega_O, W_B(q), \varepsilon_H(q)$ and $f(q)$ are the atomic volume, bare-ion pseudopotential, static Hartree dielectric function and local field correlation function, respectively.

The bare-ion pseudo-potential due to Gajjar et al., is given by [1-3]

$$W_B(q) = \frac{-8\pi Z}{\Omega_O q^2}\left(\cos(qr_C) - \frac{(qr_C)^2}{\left(1 + (qr_C)^2\right)}\right) \qquad (7)$$

Here, Z and r_C are the valence and parameter of the model potential, respectively. The details of the model potential are narrated in the literature [1-3].

Using these atomic force constants, we can generate inter atomic force constants, $K_{\alpha\beta}$, which can then be employed to investigate the elastic constants

$$\begin{aligned} K_{\alpha\beta} &= \frac{d^2\Phi(r)}{dr_\alpha dr_\beta} \\ &= \left[\delta_{\alpha\beta} - \frac{r_\alpha r_\beta}{r^2}\right]K_t + \frac{r_\alpha r_\beta}{r^2}K_r \end{aligned} \qquad (8)$$

Under the long wave phonon method, the elastic constants are studied by [1-5]

$$C_{11} = \frac{1}{12a}\sum_n N(n)\left[x^2 K^n_{xx} + y^2 K^n_{yy} + z^2 K^n_{zz}\right] \qquad (9)$$

$$\begin{aligned} C_{44} &= \frac{1}{24a}\sum_n N(n) \\ &\qquad \left[\left(y^2 + z^2\right)K^n_{xx} + \left(z^2 + x^2\right)^2 K^n_{yy} + z^2 K^n_{zz}\right] \end{aligned} \qquad (10)$$

$$C_{12} + C_{44} = \frac{1}{6a}\sum_n N(n)\left[yzK^n_{yz} + zxK^n_{zx} + xy\,K^n_{xy}\right] \qquad (11)$$

Where, a is the lattice constant and $N(n)$ is the number of atoms at the n^{th} neighbor separation.

The shear modulus C' and bulk modulus B are given by equations as follows [1-5]:

$$C' = \left[\left(\frac{C_{11} - C_{12}}{2}\right)\right] \tag{12}$$

$$B = \left[\frac{(C_{11} + 2C_{12})}{3}\right] \tag{13}$$

The extent to which the interatomic forces are non-pair wise can be obtained by investigating the breakdown of the Cauchy relation. The Cauchy ratio is obtained by using C_{12}/C_{44} .

Poisson's ratio σ is the second independent elastic parameter that is determined as [1-5],

$$\sigma = \frac{C_{12}}{(C_{11} + C_{12})} \tag{14}$$

From the calculated values of the bulk modulus and Poisson's ratio, Young modulus Y is derived as [1, 2],

$$Y = 3B(1 - 2\sigma) \tag{15}$$

In the cubic system, the propagation velocity of longitudinal and transverse waves in [100], [110] and [111] directions are given as [1-5]

$$\mathrm{v_L}[100] = \left[\frac{\mathrm{C}_{11}}{\rho}\right]^{1/2} \tag{16}$$

$$\mathrm{v_L}[110] = \left[\frac{(\mathrm{C}_{11} + \mathrm{C1}_2 + 2\mathrm{C}_{44})}{2\rho}\right]^{1/2} \tag{17}$$

$$\mathrm{v_L}[111] = \left[\frac{(\mathrm{C}_{11} + 2\mathrm{C}_{12} + 4\mathrm{C}_{44})}{3\rho}\right]^{1/2} \tag{18}$$

$$\mathrm{v_T}[100] = \mathrm{v_{T1}}[110] = \left[\frac{\mathrm{C}_{44}}{\rho}\right]^{1/2} \tag{19}$$

$$\mathrm{v_{T2}}[110] = \left[\frac{(\mathrm{C11\text{-}C12})}{2\rho}\right]^{1/2} \tag{20}$$

$$\mathrm{v_T}[111] = \left[\frac{(C_{11} - C_{12} + 2C_{44})}{3\rho}\right]^{1/2} \tag{21}$$

The behavior of phonon frequencies in the limit and independent of the direction is given by [1-5]

$$Y_1 = \lim_{q \to 0} \sum_i \frac{\omega_i^2(q)}{q^2} = \left[\frac{(C_{11} + 2C_{44})}{\rho}\right] \tag{22}$$

and

$$\mathrm{Y}_2 = \lim_{\mathrm{q} \to 0} \left(\frac{\omega_{\mathrm{T1}}}{\omega_{\mathrm{T2}}}\right)^2 = \left[\frac{(\mathrm{C}_{11} - \mathrm{C}_{12})}{2\mathrm{C}_{44}}\right] \tag{23}$$

The degree of elastic anisotropy A is the inverse of Y_2 [1-5] and given as

$$A = \left[\frac{2C_{44}}{(C_{11} - C_{12})}\right] \tag{24}$$

The value of A is unity when the material is elastically isotropic and differs from unity otherwise.

3. Results and Discussion

The constants and parameters employed for the present computational study are listed in Table 1. In the evaluation of integrals in equations (4) and (5), the upper limit of integral is taken to be 40 k_F so that a complete convergence of the model potential is achieved at higher momentum transfer and covers all oscillations of the form factor. Therefore, any artificial or fictitious cut-off in the present computations is avoided. In the present computation, the error associated will be of the order of $10^{-6} k_F / 2$. We have performed the real space sum analysis up to 33 sets of nearest neighbours in r-space, which are found sufficient for computing the elastic constants and bulk modulus using interatomic force constants to into account the long-range character for proper convergence of the calculation and to achieve desired accuracy. The present model is valid for both ordered and disordered alloys [1-8].

In the present computation, the bcc crystal structure is considered for all solid solutions. The lattice constants a are obtained from the well-known relation $(2\Omega_O)^{1/3}$. Tables 2-5 display the computed values of some static and vibrational properties of four equiatomic Rb-based binary alloys. It is noted from Tables 2-5 that our results calculated for C_{11}, C_{12}, C_{44}, $C_{12} - C_{44}$, C_{12}/C_{44} , and bulk modulus B from H-local field correction function give higher values than those obtained for the IU and S-local field correction functions. There is a good agreement for the calculated values of the Shear modulus C', deviation from the Cauchy relation, Poisson ratio σ, Young modulus Y, propagation velocity of elastic waves, phonon dispersion curves (PDC), and degree of anisotropy A using H, IU and S-local field correction functions.

Table 1: Input parameters and constants for equiatomic Rb-based binary alloys.

Metal	Z	k_F (au)	Ω_O (au)^3	r_C (au)
Li	1	0.5890	144.9	0.7738
Na	1	0.4882	254.5	1.0765
K	1	0.3947	481.4	1.3880
Rb	1	0.3693	587.9	1.4837
Cs	1	0.3412	745.5	1.9108

Table 2: Static and vibrational properties of $Rb_{0.5}Li_{0.5}$ alloy.

Properties	H	IU	S
C_{11} in 10^{10} dyne-cm^{-2}	10.98	8.01	4.53
C_{12} in 10^{10} dyne-cm^{-2}	10.26	7.17	4.00
C_{44} in 10^{10} dyne-cm^{-2}	3.63	3.89	2.83
C' in 10^{9} dyne-cm^{-2}	3.61	4.21	2.65
B in 10^{10} dyne-cm^{-2}	10.50	7.44	4.18
(C_{12}-C_{44}) in 10^{10} dyne-cm^{-2}	6.63	3.27	1.17
Cauchy's ratio (C_{11}/C_{44})	2.82	1.84	1.41
σ	0.48	0.47	0.47
Y in 10^{10} dyne.cm^{-2}	1.07	1.24	0.78
v_L [100] in 10^5 cm-sec^{-1}	2.79	2.38	1.79
v_T [100] in 10^5 cm-sec^{-1}	1.60	1.66	1.42
v_L [110] in 10^5 cm-sec^{-1}	3.17	2.85	2.24
v_{T1} [110] in 10^5 cm-sec^{-1}	1.60	1.66	1.42
v_{T2} [110] in 10^5 cm-sec^{-1}	0.51	0.55	0.43
v_L [111] in 10^5 cm-sec^{-1}	3.29	2.99	2.37
v_T [111] in 10^5 cm-sec^{-1}	1.01	1.06	0.89
Y_1 in 10^{10} dyne-cm^{-2}	12.90	11.17	7.22
Y_2	0.10	0.11	0.09
A	10.05	9.23	10.72

It is noticed from the present study that the percentage of influence of the IU-local field correction function with respect to the static H-local field correction function on vibrational properties of $Rb_{0.5}Li_{0.5}$, $Rb_{0.5}Na_{0.5}$, $Rb_{0.5}K_{0.5}$, and $Rb_{0.5}Cs_{0.5}$ is found to be 3.75%-50.68%, 2.17%-69.92%, 0%-1.08%, and 1.59%-33.44%, respectively. Such influence of the S-local field correction function with respect to the static H-local field correction function on the vibrational properties, for $Rb_{0.5}Li_{0.5}$ is 2.08%-82.35%, for $Rb_{0.5}Na_{0.5}$ is 1.45%-57.42%, for $Rb_{0.5}K_{0.5}$ is 0%-45.86%, and for $Rb_{0.5}Cs_{0.5}$ is 0%-40.36%. This clearly indicates that the local field correlations play a very effective role in explaining correctly the static and dynamic properties of such solid solutions. These static and vibrational properties of $Rb_{0.5}K_{0.5}$ solid solution computed from H and IU-local field correction functions are found to be the same.

Table 3. Static and vibrational properties of $Rb_{0.5}Na_{0.5}$ alloy.

Properties	H	IU	S
C_{11} in 10^{10} dyne-cm^{-2}	8.00	4.98	5.26
C_{12} in 10^{10} dyne-cm^{-2}	7.45	4.30	4.67
C_{44} in 10^{10} dyne-cm^{-2}	2.73	2.87	2.66
C' in 10^{9} dyne-cm^{-2}	2.78	3.43	2.96
B in 10^{10} dyne-cm^{-2}	7.63	4.53	4.87
(C_{12}-C_{44}) in 10^{10} dyne-cm^{-2}	4.72	1.42	2.01
Cauchy's ratio (C_{11}/C_{44})	2.73	1.49	1.76
σ	0.48	0.46	0.47
Y in 10^{10} dyne.cm^{-2}	0.82	1.00	0.87
v_L [100] in 10^5 cm-sec^{-1}	2.35	1.86	1.91
v_T [100] in 10^5 cm-sec^{-1}	1.38	1.41	1.36
v_L [110] in 10^5 cm-sec^{-1}	2.69	2.28	2.30
v_{T1} [110] in 10^5 cm-sec^{-1}	1.38	1.41	1.36
v_{T2} [110] in 10^5 cm-sec^{-1}	0.44	0.49	0.45
v_L [111] in 10^5 cm-sec^{-1}	2.79	2.41	2.41
v_T [111] in 10^5 cm-sec^{-1}	0.87	0.91	0.87
Y_1 in 10^{10} dyne-cm^{-2}	9.33	7.43	7.33
Y_2	0.10	0.12	0.11
A	9.83	8.39	8.98

The H-local field correction function [12] is purely static and it does not include the exchange and correlation effects. The IU-local field correction function [10] is a fitting formula for the dielectric local field correction function of the degenerate electron liquids at metallic and lower densities, which accurately reproduces the Monte-Carlo results as well as it satisfies the self consistency condition in the compressibility sum rule and short range correlations. Therefore, the IU-local field correction function influences the longitudinal phonon branches only. On the basis of IU-local field correction function [10], Sarkar et al., have proposed a simple and analytical form of the local field correction function [11].

Table 4: Static and vibrational properties of $Rb_{0.5}K_{0.5}$ alloy.

Properties	H	IU	S
C_{11} in 10^{10} dyne-cm^{-2}	6.14	6.13	4.26
C_{12} in 10^{10} dyne-cm^{-2}	5.50	5.50	3.71
C_{44} in 10^{10} dyne-cm^{-2}	2.36	2.36	2.01
C' in 10^{9} dyne-cm^{-2}	3.15	3.13	2.73
B in 10^{10} dyne-cm^{-2}	5.71	5.71	3.90
$(C_{12}$-$C_{44})$ in 10^{10} dyne-cm^{-2}	3.14	3.14	1.70
Cauchy's ratio (C_{11}/C_{44})	2.33	2.33	1.84
σ	0.47	0.47	0.47
Y in 10^{10} dyne.cm^{-2}	0.93	0.92	0.80
v_L [100] in 10^5 cm-sec^{-1}	2.17	2.17	1.81
v_T [100] in 10^5 cm-sec^{-1}	1.35	1.34	1.24
v_L [110] in 10^5 cm-sec^{-1}	2.50	2.50	2.14
v_{T1} [110] in 10^5 cm-sec^{-1}	1.35	1.34	1.24
v_{T2} [110] in 10^5 cm-sec^{-1}	0.49	0.49	0.46
v_L [111] in 10^5 cm-sec^{-1}	2.61	2.60	2.25
v_T [111] in 10^5 cm-sec^{-1}	0.87	0.87	0.81
Y_1 in 10^{10} dyne-cm^{-2}	8.32	8.31	6.34
Y_2	0.13	0.13	0.14
A	7.49	7.53	7.38

Table 5: Static and vibrational properties of $Rb_{0.5}Cs_{0.5}$ alloy.

Properties	H	IU	S
C_{11} in 10^{10} dyne-cm^{-2}	6.04	4.26	4.29
C_{12} in 10^{10} dyne-cm^{-2}	5.59	3.77	3.88
C_{44} in 10^{10} dyne-cm^{-2}	1.74	1.77	1.60
C' in 10^{9} dyne-cm^{-2}	2.26	2.43	2.05
B in 10^{10} dyne-cm^{-2}	5.74	3.93	4.02
$(C_{12}$-$C_{44})$ in 10^{10} dyne-cm^{-2}	3.84	2.00	2.29
Cauchy's ratio (C_{11}/C_{44})	3.20	2.13	2.43
σ	0.48	0.47	0.47
Y in 10^{10} dyne.cm^{-2}	0.67	0.71	0.60
v_L [100] in 10^5 cm-sec^{-1}	1.81	1.52	1.53
v_T [100] in 10^5 cm-sec^{-1}	0.97	0.98	0.93
v_L [110] in 10^5 cm-sec^{-1}	2.03	1.77	1.76
v_{T1} [110] in 10^5 cm-sec^{-1}	0.97	0.98	0.93
v_{T2} [110] in 10^5 cm-sec^{-1}	0.35	0.36	0.33
v_L [111] in 10^5 cm-sec^{-1}	2.10	1.86	1.83
v_T [111] in 10^5 cm-sec^{-1}	0.63	0.64	0.60
Y_1 in 10^{10} dyne-cm^{-2}	5.19	4.24	4.08
Y_2	0.13	0.14	0.13
A	7.73	7.29	7.80

We have also studied the PDC of four equiatomic Cs-based binary alloys viz. $Rb_{0.5}Li_{0.5}$, $Rb_{0.5}Na_{0.5}$, $Rb_{0.5}K_{0.5}$ and $Rb_{0.5}Cs_{0.5}$ along [100], [110] and [111] directions of high symmetry, which are displayed in Figs. 1-4. We have found that the phonon frequencies in the longitudinal branch are more sensitive to the exchange and correlation effects in comparison with the transverse branches. The phonon frequencies in the longitudinal branch are suppressed due to IU-local field correction and enhanced due to S-local field correction functions as compared to the frequencies due to static H-local field correction function. While in the transverse branch, the effects of exchange and correlations enhanced slightly the phonon modes. It is found that at the zone boundaries of [100] and [111] directions of high symmetry, i.e., for the larger momentum transfer, the effects of local field correlations are almost negligible. These dispersion curves do not show any abnormality in the three regions of high symmetry directions and exhibit qualitative behaviour like metallic elements.

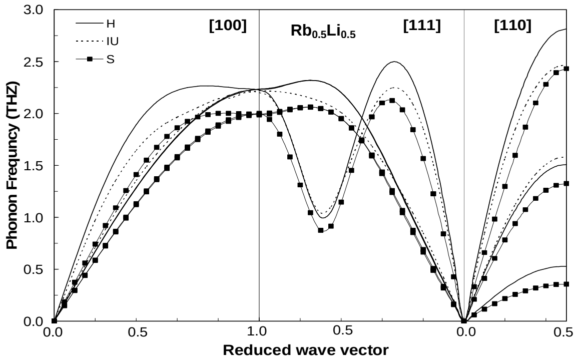

Fig.1: Phonon dispersion curves of $Rb_{0.5}Li_{0.5}$ alloy.

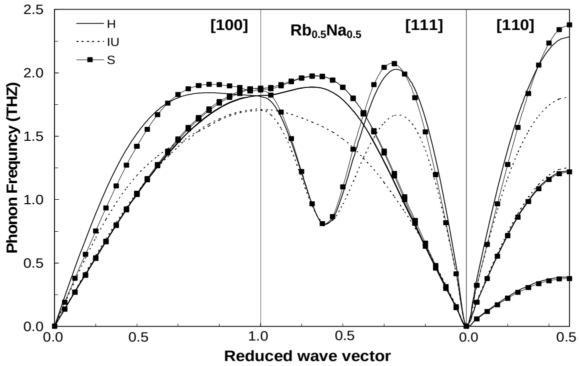

Fig.2: Phonon dispersion curves of $Rb_{0.5}Na_{0.5}$ alloy.

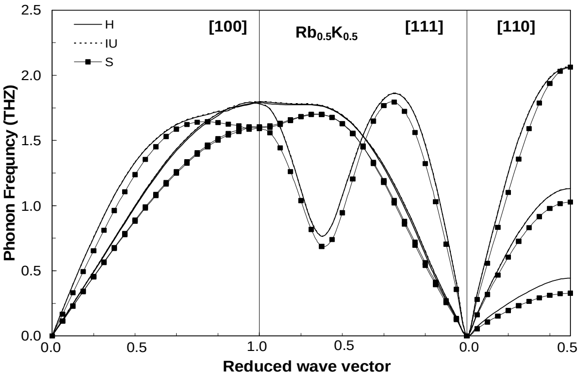

Fig.3: Phonon dispersion curves of $Rb_{0.5}K_{0.5}$ alloy.

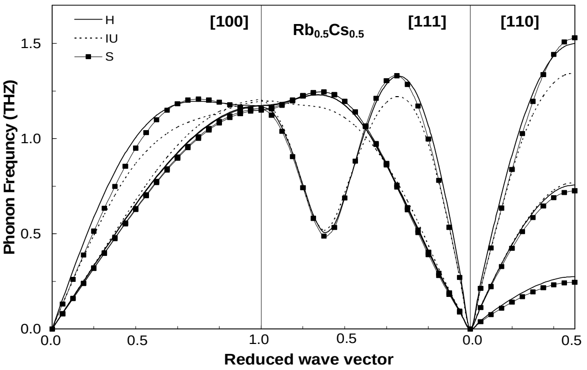

Fig.4: Phonon dispersion curves of $Rb_{0.5}Csb_{0.5}$ alloy.

The phonon frequencies computed from IU-local field correction functions diverged from static H-function in [100] [111] and [100] directions of high symmetry are about 0%-21.24%, 0%-129.95%, 0.07%-0.78%, and 0%-16.25% for $Rb_{0.5}Li_{0.5}$, $Rb_{0.5}Na_{0.5}$, $Rb_{0.5}K_{0.5}$, and $Rb_{0.5}Cs_{0.5}$ solid alloys, respectively. While the phonon frequencies computed from S-local field correction functions differed from static H-function in [100], [111] and [100] of high symmetry directions are 0%-99.19% for $Rb_{0.5}Li_{0.5}$, 0%-142.92% for $Rb_{0.5}Na_{0.5}$, 0.63%-144.88% for $Rb_{0.5}K_{0.5}$, and 0%-13.22% for $Rb_{0.5}Cs_{0.5}$ solid solutions.

Also, we observed from the PDC that, when we move from $Rb_{0.5}Li_{0.5} \rightarrow Rb_{0.5}Cs_{0.5}$ alloys, the phonon frequency decreases with an increase in the average volume of the solid alloys. The experimental phonon frequencies of such alloys are not available in the literature for further comparison and remarks. But, in the absence of experimental information, such calculations may be considered as one of the guidelines for further investigations, either theoretical or experimental. Hence, such a study could be extended for the other types of binary alloys.

4. Conclusions

We concluded that the present model is successful in explaining the static and vibrational properties of equiatomic Rb-based binary alloys and hence it could be explored for predicting the behavior of other such solid solutions. The comparison of present theoretical findings helps us note that the binding of $A_{1-X}B_X$ (A = Rb and B = Li, Na, K, Cs) is comparable with pure metals and hence behaves like a solid metallic alloy. This can be confirmed by investigating its total crystal energy and heat of solution. Such study is under progress and the results shall be reported in due course of the time. From the present study, we conclude furthermore that it should be interesting to apply other local pseudopotentials for such comprehensive study in order to judge and confirm its wider applicability.

References

[1] P. N. Gajjar, A. M. Vora, M. H. Patel and A. R. Jani, Different Disordered – Systems, Eds. Furukawa et al., INDIAS Publ., Allahabad (India) (2000) p.57.

[2] Aditya M. Vora, J. Phys. Chem. Sol. **68**, 1725 (2007); Chinese Phys. Lett. **25**, 654 (2008); Front. Mater. Sci. China **2**, 311 (2008); Fizika A **17**, 87 (2008); Moroccan J. Conden. Mat. **10**, 7 (2008).

[3] P. N. Gajjar, M. H. Patel, B. Y. Thakore and A. R. Jani, Commun. of Phys. **12**, 81 (2002).

[4] P. N. Gajjar, B. Y. Thakore, H. K. Patel and A. R. Jani, Acta Phys. Pol. **A88**, 489 (1995).

[5] P. N. Gajjar, B. Y. Thakore, J. S. Luhar and A. R. Jani, Physica B **215**, 293 (1995).

[6] R. F. Wallis, A. A. Maradudin, A. G. Eguiluz, A. A. Quong, A. Franchini and G. Santara, Phys. Rev. B **48**, 6043 (1993).

[7] T. Soma, H. Ohsugi and H. Matsuo Kagaya, Phys. State. Sol. (b) **124**, 525 (1984).

[8] W. A. Kamitakahara and J. R. D. Copley, Phys. Rev. B **18**, 3772 (1978).

[9] Y. A. Chushak and A. Baumketner, Euro. Phys. J. B **7**, 129 (1999).

[10] S. Ichimaru and K. Utsumi, Phys. Rev. B **24**, 7385 (1981).

[11] A. Sarkar, D. S. Sen, S. Haldar and D. Roy, Mod. Phys. Lett. B **12**, 639 (1998).

[12] W. Harrison, Elementary Electronic Structure, (World Scientific, Singapore, 1999) p.462.

Received: 29 January, 2010
Accepted: 16 July, 2010