ISSN NO. 2320-5407

*Journal homepage: http://www.journalijar.com*

*INTERNATIONAL JOURNAL OF ADVANCED RESEARCH*

**RESEARCH ARTICLE**

# Lattice Dynamics of RbCl and RbBr under Compression

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## *Manuscript Info*

***Manuscript History:***

Received: 11 April 2013
Final Accepted: 03 May 2013
Published Online: May 2013

***Key words:***
TSM,
Phonon dispersion curves,
Phonon density of states,
phase transition.

## *Abstract*

Lattice dynamics of RbCl and RbBr have been investigated at high pressure using three body forces shell model. The phonon dispersion curves are derived at 1 atm and at high pressure (close to the phase transition pressure). Good agreement is obtained between the theoretical and experimental data for dispersion curves of RbCl and RbBr. We have also calculated the one phonon density of states at high pressure near to the phase transition pressure for RbCl and RbBr.



## Introduction

The phonons in condensed Matter physics have played a crucial role, since there discovery by Einstein, at the beginning of the century. The pioneering work of Birdgman[1, 2]opened an area of research which deals with the generation of very high pressure and measurements of the properties of matter under pressure.

We know that, the theoretical and experimental determination of lattice vibration and phonon properties of solids is important research field, because these field have an important effect on the acoustic, Electrical, Optical, Mechanical and thermal properties etc. [3-9]. Several theories are available for determination of phonon properties and lattice vibration of solids, such as Rigid ion model, Shell Model, Deformation Dipole and Shell Model, Breathing Shell model and Microscopic Theories of Lattice Vibration etc.[10-15].

Recently, K Haddadi et al[16] have calculated the structural, elastic, and high-pressure properties of RbX (X=Cl, Br, F, I) and N.C.Payper et al[17] have determined the cohesive energy of three phases of solid cubic rubidium chloride (RbCl), the zinc blend structured 4:4 phase, the 6:6 sodium chloride polymorph and the 8:8 phase with the cesium chloride structure.

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In the present work have been calculate the dynamical properties of solids at high pressure with the view to get an insight into the phenomena of phase transition governed by dynamic excitation such as phonons. Complete phonon spectrum of nonmetallic ionic solids RbCl and RbBr have been calculated using Three body force shell model (TSM) both at ambient pressure as well as at high pressure close to the phase transition pressure of corresponding solid. One phonon density of states of these solids have also been calculated at different pressure up to the phase transition pressure.

## Material and Methods

In order to describe the phonon dispersion curves of Rubidium compounds (RbCl and RbBr), we use a three-body force shell model (TSM) discussed by Singh and Verma[18] .This mechanism causes a transfer of charge between the overlapping ions. In turn, these transferred charged interact with all other charges via their associated Coulomb field and give rise to Long Range (LR) many body interactions whose most significant component in the TBI (Three-body interaction). The introduction of this TBI in the framework of RSM (Rigid Shell Model) [19] has given rise to TSM of Singh and Verma[18]

The dynamical matrix corresponding to TSM can be write as,

$$D(\vec{q}) = (R + Z_m C' Z_m) - (R + Z_m C' Y_m)(K + R + YmC'Ym - 1RT + YmC'Ym) \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots 1$$

In the equation (1) R and T represent the modified short-range core-core and core-shell interaction matrices.

where $Y_m$ and $Z_m$ are (6x6) diagonal matrices for the modified ionic charge and shell charges. here, C' is the modified LR Coulomb matrix, such that

$$C' = C + \frac{Zr_{0f0}}{Z_m^2} V \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots 2$$

here C is the usual coulomb matrix evaluated by Kellerman [20] and V is the TBI matrix (6x6) with its elements [21].The value of TBI matrix elements have been listed ref.[21].

For making our calculation especially at high pressure, we have made use of seven parameters. First six include short-range force constants while the last one is $Z_m$. The above equations relating to the macroscopic properties with the model parameters are already available in literature [21]. Input constants used to calculate the model parameter for RbCl and RbBr area taken from references [22] .The input constants for RbCl and RBr have been reported in Table 1.

## Result and Discussion

Phonon dispersion Relation has been calculated using the model parameter listed in Table 2. The phonon dispersion curves derived from TSM at 1 atm and at high pressure (close to the phase transition pressure) for RbCl and RbBr have been displayed in fig.1-2 respectively. This enable us to judge the effect of pressure on different phonon modes in symmetry direction solid line in fig1-2 represent the result at 1 atm pressure. A glance at dispersion curves given in fig1-2 reveals excellent agreement between theoretical and experimental result at 1 atm pressure [23, 24] for RbCl and RbBr.

To obtain the complete phonon spectra, the secular determinant has been solved for all the 48 non-equivalent point of the first Brillouin zone out of the total 10×10×10=10000 points. These gives 6000 frequencies represent with proper statistical weights taken into account. These frequencies represent the complete vibrational spectra (see kellerman [25]).For the calculating the phonon density of states the whole frequency spectrum has been divided into small intervals. A plot is made between the no. of frequencies that lie in a given frequency interval and the corresponding frequency interval. This plot gives the frequency spectrum. One phonon density of states calculated near phase transition pressure for RbCl and RbBr have been displayed in fig.3-4, respectively.

In the absence of the phase transition, the phonon frequencies are expected to increase with the application of hydrostatic pressure. This is because the atoms brought closer to each other under compression and hence they sit in steeper potential wells. This is termed as normal behavior of phonon under pressure. However, often one encounters a few phonons, which show the opposite behavior i.e. the frequency of some phonon modes decreases with increase in pressure. A decrease in frequency implies a reduction in corresponding force constant, which in turn has connected to elastic constants. The phonon which exhibit decrease in frequency with increasing pressure is called a soft phonon as it leads to softening of the lattice. This also point towards instability of the crystal structure leading to phase transition.

In conclusion, we have calculated the pressure dependence of the phonon dispersion curves and phonon density of states of RbCl and RbBr using three body force shell model (TSM). It is observed that the energies of the optical phonons (both longitudinal and transverse) as well as longitudinal acoustic phonons increase with pressure. The energies of the transverse acoustic phonons decrease or soften with pressure. Phonon density of state calculated up to the phase transition pressure of corresponding solid, show pronounced shift in the frequency spectrum with pressure. Since no information about phonon frequency was used in calculating the model parameters, the good agreement with experiment and obtained at ambient pressure give one confidence in the predictions made for the phonon properties of RbCl and RbBr at none zero pressure.

**Table .1 Input constants for the calculation of model parameters at ambient pressure:**

| Solids | $C_{11}$(GPa) | $C_{12}$(GPa) | $C_{44}$(GPa) | $r_o$($A^o$) |
|---|---|---|---|---|
| RbCl | 44.99[a] | 6.70[a] | 4.92[a] | 3.29[a] |
| RbBr | 33.63[a] | 4.70[a] | 4.09[a] | 3.44[a] |

[a]Ref. [22]

**Table 2.Model parameters for RbCl and RbBr**

| Solids | RbCl | | RbBr | |
|---|---|---|---|---|
| Parameters | 1 atm(0.0GPa) | 0.9Gpa | 1 atm(0.0Gpa) | 0.9 Gpa |
| $A_{12}$ | 12.4108 | 13.9166 | 11.0745 | 13.6329 |
| $B_{12}$ | -0.9563 | -1.0973 | -0.84411 | -1.0066 |
| $A_{11}$ | -.0.0837 | -0.0776 | -0.08463 | -0.08461 |
| $B_{11}$ | 0.0197 | 0.0202 | 0.01544 | 0.01625 |
| $A_{22}$ | 0.15447 | 0.23134 | 0.16246 | 0.28305 |
| $B_{22}$ | 0.02366 | 0.02066 | 0.0323 | 0.02804 |
| $Z_m$ | 0.9940 | 0.9931 | 0.9911 | 0.894 |

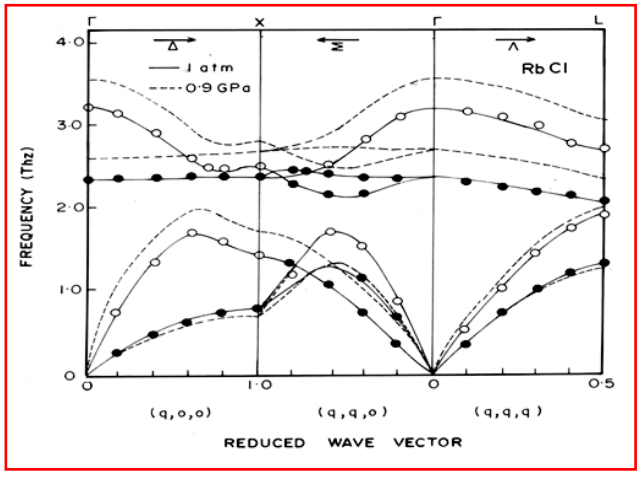


**Fig.1: Dispersion curves for RbCl. Solid Lines –result at 1 atm., dashed lines result at 0.9GPa. Experimental points (ref.23) (○-longitudinal, ●-transverse)**

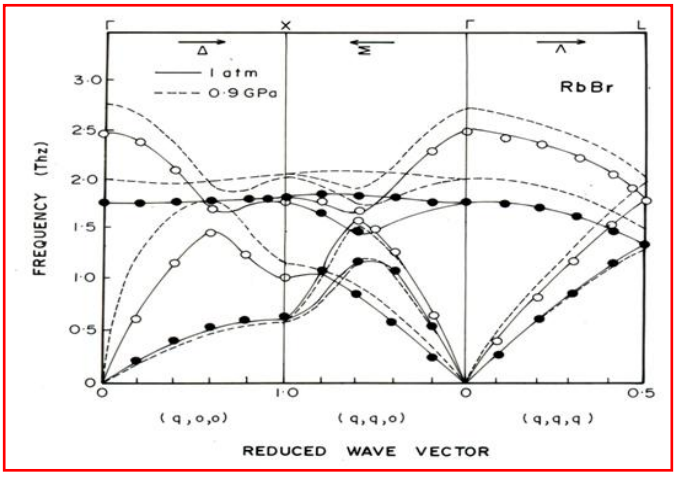


**Fig.2: Dispersion curves for RbBr. Solid Lines – result at 1 atm., dashed lines result at 0.9GPa. Experimental points (ref.24) (○-longitudinal, ●-transverse)**

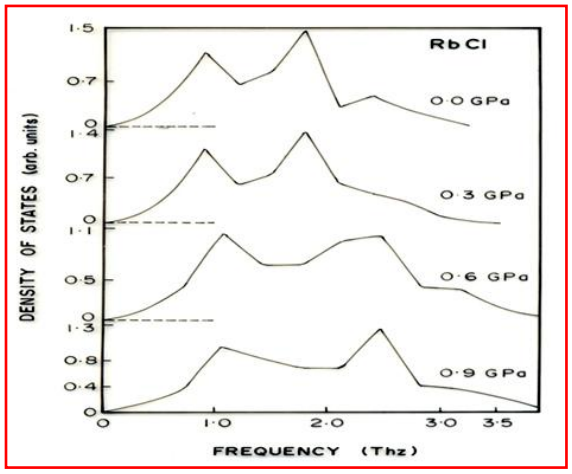


**Fig.3: Calculated one phonon density of states of RbCl close to the phase- transition pressure.**

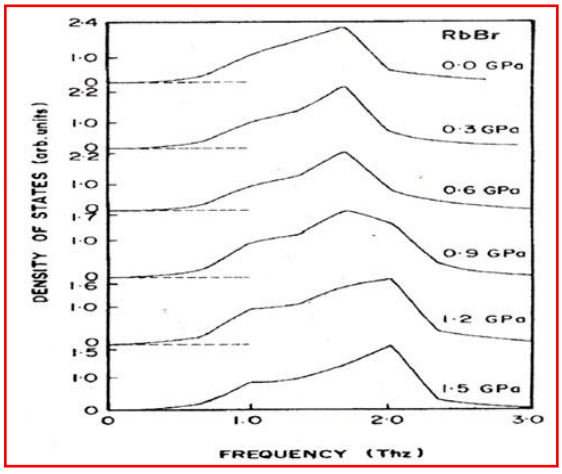


**Fig.4: Calculated one phonon density of states of RbBr close to the phase- transition pressure.**

## References:


1. Collected paper of P.W. Bridgman**, Vol -7** *Harvart univ. press, Cambridge, mass* (1964).

2. P.W. Bridgman, High *Pressure Engineering, The institution of mechanical engineers (London)***182**, Part 3C (1968).

3. Subrata Ghose, Michal Krisch, Artem R.Oganov, Alexander Beraud, Alexey Bosak, Revansidha Gulve, Raghunandan seelaboyina, Hexion Yang, and Surendra K. Saxena *Phy.Rev. Letter*, **96**, 035507(2006).

4. R. Mittal and S. L. Chaplot *BARC Nwes letter no.***249** (2003).

5. R. Mittal, L. Pintschovius, D.Lamago, R. Heid, Bohnen, D. reznik, S.L. Chaplot, Y. Su, N. Kumar, S. K. Dhar, A. Thamizhavel and Th. Brueckel *Phy.Rev. Letter*, **102**, 217001 (2009).

6. Graeme Achland *RIKEN Review no.***29** (2000).

7. Y. F. Guo, H. F. Zhang, H. B. Liu, D.L. Zhao and C.Y. Wang *Computational Material Science*, **20**,228(2001).

8. Sefa Kazanc and Soner Ozgen, *Turk J. Phys*. **32**, 315-322 (2008).

9. Wilfried, B.Holzpfel, Z.Naturforsch, **63b**, 718-724 (2008).

10. E. W. Kellerman *Phil Trans. Roy Soc. (Londn)* **A230-A238**, 513 (1940).*Proc R.Soc.(Lond.)* **A178**, 17 (1941).

11. B.G. Dick and A.W.Overhauser. *Phys. Rev*.**112,** 90,(1958)

12. W.Cochran, Z.Krist *Phys.Rev. Lett*., **2**, 495 (1959).

13. A.D. Woods, W.Cochran and B.N.Brockhouse *Phys. Rev*. **119**, 980 (1960).

14. J.R.Hardy *Phil Mag.***4** 1278(1959):**6**, 27, (1959) :**7**, 315, (1959).

15. M. S. Kushwaha and S.S. Kushwah *J.Phys. Chem*., **41**, 484,(1980).

16. K. Haddadi, A. Bouhemadou, L. Louail, D. Maouche *Phase Transitions: A Multinational Journal***, 82**, 3, 266-279 (2009).

17. N. C. Payper, A. L. Kirkland and J H. Harding *Journal of phys. Cond. Matt*. **18,** 983, (2006).

18. R.K. singh and M.P. Verma, *Phys. Sol (b)*, **33**, 769 (1969).

19. A.D.B. Wood, W.Cochran and B.N.Brockhouse, *Phy.Rev*. **119**, 980, (1960).

20. E.W.Kellerman Phil Trans. Roy Soc. (Londn) A230-A238, 513 (1940).Proc R.Soc.(Lond.) A178, 17 (1941).

21. R.K. Singh ,Phys. Reports., Netherlands, 85,259, (1982), and references therein.

22. J.R. Hardy and A.M. Karo, *The lattice dynamic and statics of alkali Halide Crystal Plenum, New York*, (1979).

23. G.Raunio and s. Rolandson *J. Phys.* **C3**, 1013 (1970).

24. G.Raunio and s. Rolandson *J. Phys*. **C4**, 958 (1971).

25. E.W. Kellermann, *Phys. Trans Roy.Soc. (Lond.)* **A238**, 513 (1940), *Proc. R.Soc.(Lond.)* **A178**, 17 (1941).