SGVU J CLIM CHANGE WATER
Vol. 1(1), Jan 2014 pp 57-61
ISSN: 2347-7741

PHONONS IN BODY CENTERED CUBIC NIOBIUM-MOLYBDENUM ALLOY

RAMA NAND SHARMA[1]* DR. S.B.L TRIPATHY[2]
[1]*Lecturer in Physics, Government College, Neem Ka Thana, Rajasthan, India*
[2]*Prof. Department of Higher Education, Directorate College Education, Jaipur, India*
**Corresponding Author, email:*

Abstract - The phonon dispersion relation entailing from the solution of secular equation are compared with the recent experimental findings on the bcc alloy, the two body form of Morse potential. The Lattice dynamics Nb-Mo alloy computed is well matched with our extensively modified exponential potential (EMEP) computed results, Our recent study describes successfully in reproducing anomalous features of dispersion curve for Nb-Mo system.

Keywords - Bcc, Phonons, Extensively modified exponential Potential (EMEP), Morse Potential, phonon dispersion, secular equation.

INTRODUCTION

The lattice dynamical behavior of transition metals has been studied on the basis of two different approaches, i.e. pseudo potential. The former studies [1-4] involve dynamics of non various simplifying assumptions for discussing the crystal dynamics of non simple metals. These model potentials require further modifications with respect to their non-centrality and dielectric functions for yielding a good comparison between the computed and experimental dispersion date. The later studies [5-8] of these metals suffer from the deficiency of lattice instability and use extensive fitting procedures. Not only this, the first principle theories [9-11] to the lattice dynamics of transition metals make use of drastic approximation to arrive at useful conclusions and increase computer time many times.

The normal modes of vibration in a Mo-Ru alloy were measured using inelastic neutron scattering. The resulting frequency wave vector dispersion relations are compared with the pure Mo results of Powell, Martel and Woods. The phonon dispersion curves of transition metals and alloys have been the subject of a number of theoretical and experimental investigations. The electronic structures of the column V and column VI metals differ in that the column V and Column VI metals differ in that the Column –V metals have five electrons outside the closed shell and the column VI metals.

The phonon dispersion Curves of a series of binary alloys of metals in Column V and VI in the same row should provide information on how the addition of d-electrons to the unfilled shell changes the normal modes of vibration and, hence, the inter atomic force system. The alloy system chosen for these computations was the niobium-molybdenum system, both metals belonging to the 4d series.

The pure metals have excellent neutron properties and extensive computation of their dispersion relations, the metals from a complete series of disordered solid solutions, all having a body centered cubic structure, thus permitting inter comparisons to be readily made. Four modified and simplified version of the shell model due to Fielex are developed to describe the dispersion relation in tantalum and niobium.

The models (model 1 , 2 , 3) thus developed adequately account for the niobium. Cauchy's discrepancy, and anisotropy exhibited by the metals.

It is found that the interactions coupling the nearby d-shells are effectively angular for tantalum and central pair wise for niobium.

The lattice dynamical models described above may now be used to various properties of Nb-Mo alloys, particularly those which are directly related to the phonon frequency distribution function. This function has been calculated from the Born-Von karman models using the method of Gilat and Raubenheimer[15]

The normal modes of vibration of the column-V and VI transition metals niobium[16] and molybdenum[17] show striking differences. These imply widely differing inter-atomic forces in the metals, and are attributed to their different electronic structures. We have computed phonon dispersion curve of $Nb_{0.44}M_{0.56}$ alloy be mean of extensively modified exponential potential (EMEP). The phonon frequency was computed by the technique of coherent, inelastic neutron scattering for the alloy.

Theoretical dispersion curve is confined to the higher symmetry direction only [100], [111] and [110].

Thus 12th neighbors is the most distant atomic neighbor. Whose atomic force constant can be determined from these measurements[18]. Analysis of the dispersion curve in terms of inter planer force constant Powell et.al. [19] showed the "effective forces" in these transition metals and alloys to be of very long range however, this 12th neighbors extensively modified exponential potential (EMEP) model describes the overall features of the dispersion curve.

METHODS

The phonon frequencies along the major symmetry directions have been computed defined by equations (2) to (8) for $Nb_{0.44}$-$Mo_{0.56}$ alloy. For thriving at the phonon frequencies along the major symmetry directions, the following secular determinant is solved i.e

$$! \, d \, \alpha\beta \, (q) - 4\pi^2 \, M \, v^2 \, I \, ! = 0 \qquad (1)$$

Where I is the unit matrix of 3x3 order and M is the mass of the atom. The phonon-dispersion relation. So obtained may be expressed as

along [100], $q_\alpha = q$, $q_\beta = q_\gamma = u$

$$4\pi^2 M \upsilon^2_L = | \, D_{\alpha'\alpha'} (q) \, |_{[100]}$$

$$= (16/3)\,\beta_1 \sin^2(aq/4) + 4\,\beta_2 \sin^2(aq/2) \qquad (2)$$

$$4\,\pi^2 M \upsilon^2_T = | \, D_{\beta'\beta'} (q) \, | \, [100]$$

$$= (16/3)\,\beta_1 \sin^2(aq/4) \qquad (3)$$

along [110], $q_\alpha = q_\beta = q / v\,2$ $q_\gamma = 0$

$$4\pi^2 M \upsilon^2_L = | \, D_{\alpha'\alpha'} (q) + D_{\alpha'\beta'} (q) \, |_{[110]}$$

$$= [\,(16/3)\,\beta_1 + 4\,\beta_2\,] \sin^2(aq/2v\,2) \qquad (4)$$

$$4\pi^2 M \upsilon^2_{T_1} = | D_{\alpha'\alpha'}(q) - D_{\alpha'\beta'}(q) |_{[110]}$$

$$= 4\beta_2 \sin^2(aq / 2v\ 2) \quad (5)$$

$$4\pi^2 M \upsilon^2_{T_2} = | D_{\gamma'\gamma'}(q) |_{[110]}$$

$$= (8/3)\beta_1 \sin^2(aq / 2v\ 2) \quad (6)$$

along [111], $q_\alpha = q_\beta = q_\gamma = q / v\ 3$

$$4\pi^2 M \upsilon^2_L = | D_{\alpha'\alpha'}(q) + 2 D_{\alpha'\beta'}(q) |_{[111]}$$

$$= (4\beta_2 + 8\beta_1)\sin^2(aq / 2v\ 3) + \frac{16}{3}\beta_1 \sin^2(aq / 4v\ 3)$$

$$- 16\beta_1 \sin^2(aq / 2v\ 3)\ \sin^2(aq / 4v\ 3) \quad (7)$$

$$4\pi^2 M \upsilon^2_T = | D_{\alpha'\alpha'}(q) - D_{\alpha'\beta'}(q) |_{[111]}$$

$$\frac{16}{} \beta_1 \sin^2(aq / 4v\ 3) + 4\beta_2 \sin^2(aq / 2v\ 3) \quad (8)$$

RESULT AND DISCUSSION

A machine program was developed on the theoretical lines given in the preceding section and the same was fed to the computer to obtain to the result given in tables 1. The present study considers the 228 atoms extending to 12th neighbors to compute phonon frequency. The computed phonon frequencies along with the calculated data of B.M. Powell et.al[20]. Figures 1. depicts the computed phonon dispersion curve indicated by (-----) for the bcc binary alloy $Nb_{0.44}$-$Mo_{0.56}$ respectively. Marking (®,0) on the corves show the experimental data reported by B.M. Powell et.al. The phonon frequencies given by the extensively modified exponential potential (EMEP) aggress reasonably well with the measured data for almost all the bcc binary alloy studied along the major symmetry direction. However, we present below a critical analysis of over computed results with reference to measured data for each bcc binary alloy studied.

The data presented here will hopefully clarify the emerging theoretical situation. The choice of Nb-Mo. as the alloying constituents essentially removes mass effects as a confounding variable. A Born-Von Karman model was not adequate in explaining the only significant different in feature between the pure metals and alloys. Indeed, the original Born-Von Karman fit to pure Nb-Mo alloy by Powell et.al[20] was already marginal. A proper theoretical treatment must include long-long electronic effects. The interpretation of the neutron results indicates the possibility of correlating the behavior of the dispersion curves of the complete $Nb_{0.44}$ $Mo_{0.56}$ system in-terms of a

rigid-band structure on this picture, the alloys can be considered to have electronic and phonon structures, analogous in these respects to pure metals.

Table 1 Computed phonon frequincies (x 10^{12} Htz.) For $Nb_{0.44}$ $M_{0.56}$ alloy
M = 15.7044 x 10^{-26} Kg. and a_0 = 1.6080 x 10^{-10} m

	100		111		110		
q/qmax	L	T	L	T	L	T_1	T_2
0.1	1.2023	0.5081	4.7513	1.2097	1.5126	0.4871	1.0021
0.2	2.2530	1.6309	6.1055	2.6172	3.0051	0.9715	1.7550
0.3	3.7563	2.9717	6.3029	3.7660	4.7023	1.5022	2.5012
0.4	4.6012	3.8058	5.7541	4.8339	6.0010	2.2035	3.6120
0.5	5.7592	4.7513	5.2015	5.6504	6.9543	2.6561	4.7511
0.6	6.4558	5.6951	5.2597	6.4885			
0.7	6.8022	6.3199	5.7418	6.4885			
0.8	7.0715	6.7462	6.5214	6.7719			
0.9	7.1529	7.0060	6.9527	7.0536			
1.0	7.2534	7.2534	7.2534	7.2534			

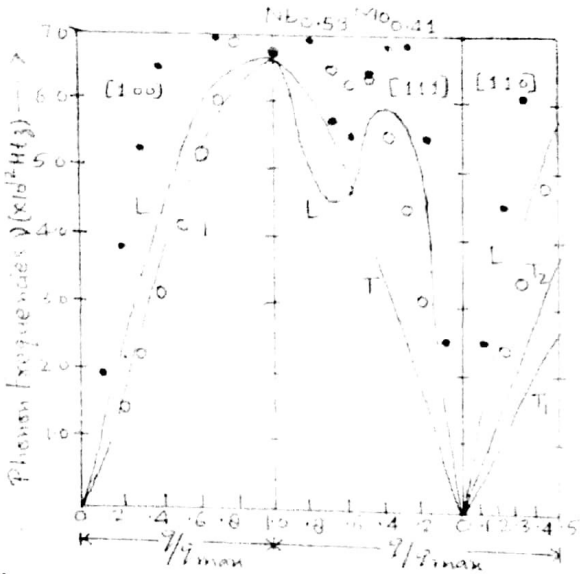

Figure 1. Phonon dispersion curve of bcc Nb. 44 Mo .56 alloy present study; (0.0) experimental findings from powell et.all[15].

CONCLUSION

The phonon dispersion curve in bcc alloy are notoriously full of anomalies [21]. It is only recently that these anomalies have been accounted for in a satisfactory way to some extent. Previous to devise potentials have met with a limited success[22] and it is not surprising to find discrepancies as high as 100% between the computed and experimental phonc.. frequencies in the literature. In this light, a comparison of the experimental[19] extensively modified exponential potential (EMEP). However, the difference of 10% to 30% between the presently computed phonon frequencies and the measured frequencies[19] can be further reduced by explicit inclusion of appropriate three forces and the suitable electronic contribution in a more direct manner. Anyway, our results are free from the relative standard error and this fact enhances the reliability[23] of our model.

REFERENCE

JA. Moriarty, Phys. Rev. B1, 1362 (1970): ibid.6, 1239 (1972)

B.A. Oli, A.O.E. Animalu, Phys. Rev. B 13, 2398 (1976)

O.P. Kulshrestha, J.C. Upadhyaya, Ind. J Pure. Appl. Phys. 14, 253 (1976)

J. Singh, N. Singh, S. Prakash, Phys. Rev. B 12, 3166 (1975)

L.A. Bertolo, M.M. Shukla, J. Phys. Soc. Jpn. 38, 1439 (1975)

C.M. Goel, B.P. Pandey, B. Dayal, Phys. Status solidi B66, 759 (1974)

J. Prakash, I.P. Pathak, M.P. Hemkar, Aust. J. Phys. 28, 57 (1975)

P.K. Sharma, R.N. Awasthi, Phys. Rev. B18, 1963 (1979)

S.Nand, B.B. Triapthi, H.C. Gupta, J.Phys. Soc. Jpn. 41, 1237 (1976)

J.C. Upadhyaya, L. Dagens, J. Phys. F8, L-2 (1978).

R. Rebonato. J.Q. Broughton, Philos. Mag. Lett. 55, 225 (1987)

S.K. Sinha, Dynamical Properties in solids Vol. III ed. G.K. Horton and A.A. Maradudin (New York, North Holland) (1979)

H.G. Smith, N. Wakabayashi and M.Mostoller, Super Conductivity in d- and F-banch metals [2nd Roch conf.] ed. D.H. Douglas [New York, Plenum], P. 223 (1976).

R.N. Khanna and R.P.S. Pathore, Phys. Status sol. (b), 107, 346 (1981)

G. Gilat and L.J. Raubenheimber, Phys. Rev. 144, 390 (1966)

Y. Nakagawa and A.D.B woods., Phys. Rev. Lett. 11, 805 (1963)

A.D.B. Woods and S.H. Chen, Solid State commun. 2, 233 (1964)

G.L. Squires, In elastic Scattering of neutrons in solids and liquids, vol. II, IAEA, Vienna, P. 171 (1963)

B.M. Powell, P. Martel and A.D.B. Woods, Phys. Rev. 171, 727 (1968)

B. .M. Powell, P. Martel and A.D.B. Woods, Can. J. Phys. 55, 1601 (1977)

S.T. Chui, Phys. Rev. B9, 2097 (1974)

A.O.E. Animalu, Phys. Rev. B8, 3555 (1973): K. Terakura, J. Phys. F14, 3255 (1981)

R.S. leigh, B. Szigett, V.K. Tewari, Proc. R.Soc. Lond. A32.