Phonon dispersion of bcc transition metals using the temperature-dependent pair potential

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(Received 13 February 1989)

The phonon dispersions of body-centered-cubic transition metals are calculated with use of the fast-converging temperature-dependent pair potential proposed by the authors recently [Phys. Rev. B **38**, 7415 (1988)]. The calculated results for group-V*a* and -VI*a* elements have been compared with existing experimental results and commented on.

There exist several phenomenological and first-principles theories to study the lattice dynamics of transition metals.[1–4] Recently the authors[5] have proposed a temperature-dependent pair potential for transition metals and have calculated the phonon dispersion curves, elastic constants, and binding energy for a number of fcc transition metals and bcc iron. The calculated results have been found in good agreement with experimental values for all the metals. For bcc transition metals, the phonon dispersion curves are notoriously full of anomalies.[6,7] It is only recently that these anomalies have been accounted for in a satisfactory way.[8] Previous attempts to devise potentials for bcc transition metals have met with limited success,[9,10] and it is not uncommon to find discrepancies as high as 100% between calculated and experimental frequencies in the literature. In this light, comparison of the experimental[11–14] and present calculated phonon dispersion curves using a damped pair potential are quite encouraging.

The effective valence Z, number of electrons in a d-band, Z_d, and the d-state radius r_d are taken to be the same as those given in Ref. 15. The electron-density parameter r_s at room temperature is taken corresponding to the observed volume.[16] These are listed in Table I for convenience. The empty-core model potential parameter r_c is determined by matching the transverse mode of phonon spectra in the long-wavelength region with the observed value in the [100] direction. The values of r_c so obtained are given in Table I. Figures 1–5 show the phonon frequencies of V, Nb, Ta, Mo, and W, respectively, as a function of the reduced wave vector as obtained with Eqs. (8)–(18) and (23) of Ref. 5. The contributions up to seventh shell have been found sufficient to achieve convergence for these calculations. All the calculated curves exhibit the same qualitative structure with maxima and minima located approximately at the same values of reduced wave vector. For the metals of group V*a* (V,Nb,Ta) the agreement with experimental values is reasonable good in all the symmetry directions except in [110]L and [110]T branches for V and Nb, respectively. The maximum discrepancy at zone boundary in the [110]L branch for V, Nb, and Ta is found to be 72%,

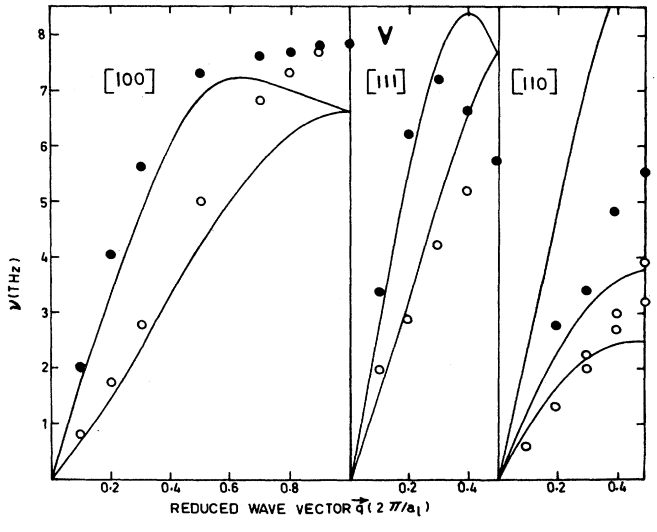

FIG. 1. ω vs **q** for V. The solid lines represent the calculated results of phonon dispersion curves at 300 K along major symmetry directions. The points are the experimental values. Here, a_l is the lattice parameter.

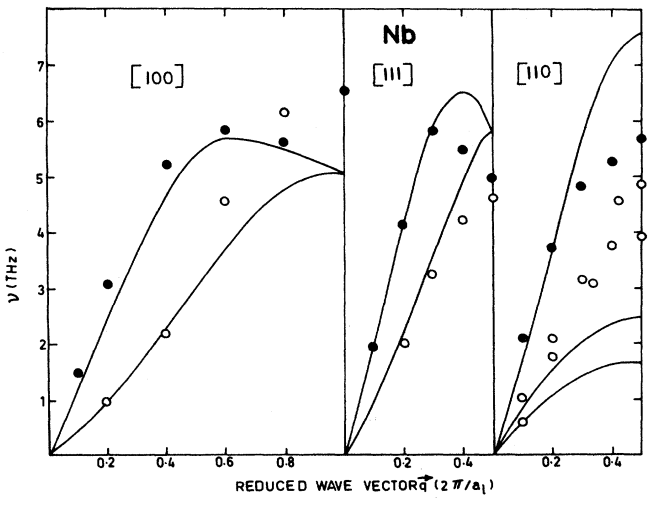

FIG. 2. Same as Fig. 1, but for Nb.

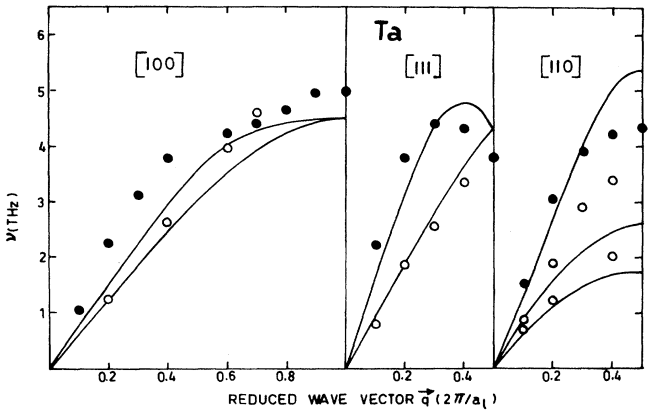

FIG. 3. Same as Fig. 1, but for Ta.

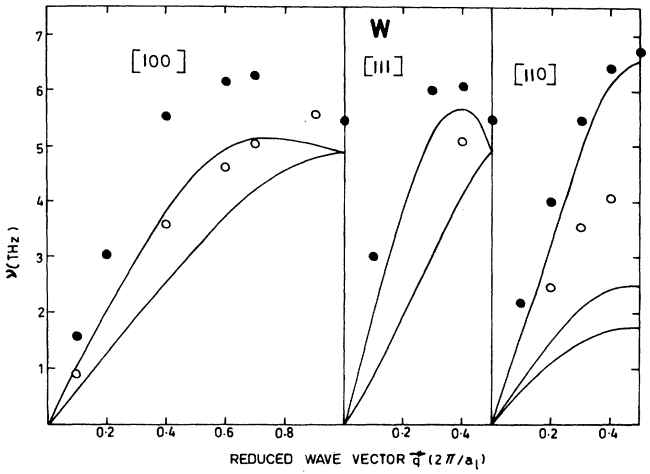

FIG. 5. Same as Fig. 1, but for W.

33%, and 25%, respectively. It should be remembered that these group-V*a* metals present additional anomalies in their dispersion curves throughout the Brillouin zone,[12] such as upward concavity at the origin of the [100]T and [110]T_2 branches, with the subsequent crossing of the [100]L and [110]L curves. For the metals of group VI*a*, on the other hand, the agreement with experimental[12,14] values is not so good. However, the calculated values are in reasonably good agreement with experimental values for [100]T, [111]L, [111]T, and [110]L modes of Mo and for [111]L and [110]L modes of W. It is to be noted that phonon dispersion curves for these metals shift downwards by increasing the potential parameter r_c beyond the values reported in Table I. Furthermore, for Mo and W the maximum frequency to occur for the [110]L mode is correctly predicted to be similar to the values obtained by Rebonato and Broughton[4] using the Finnis-Sinclair potential.[17] Only the tight-binding method[18] in the second-moment approximation, amongst the (semi)phenomenological models known to authors, gives comparable overall agreement with experimental phonon dispersion curves. It predicts incorrectly, however, the elastic constants.

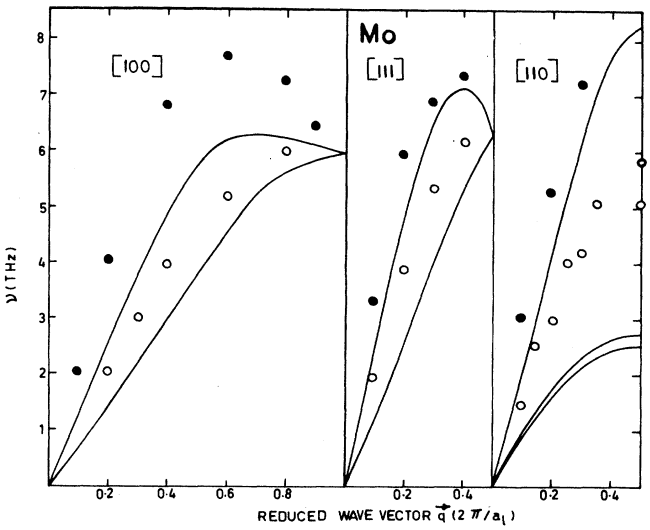

FIG. 4. Same as Fig. 1, but for Mo.

The authors acknowledge financial assistance from Maharshi Dayanand University, Rohtak.

TABLE I. Observed (Ref. 16) electron-density parameter r_s and fitted values of the pseudopotential parameter r_c.

	$_{23}$V	$_{41}$Nb	$_{73}$Ta	$_{42}$Mo	$_{74}$W
r_s (a.u.)	2.461	2.675	2.675	2.560	2.576
r_c (a.u.)	1.930	2.280	2.090	2.150	2.200

[1]S. Prakash and S. K. Joshi, Phys. Rev. B **2**, 915 (1970); **4**, 1770 (1971); **5**, 2880 (1972).
[2]W. Hanke, Phys. Rev. B **8**, 4585 (1973).
[3]J. A. Moriarty, Phys. Rev. B **1**, 1362 (1970); **6**, 1239 (1972); **6**, 2066 (1972).
[4]R. Rebonato and J. Q. Broughton, Philos. Mag. Lett. **55**, 225 (1987).
[5]N. Singh, N. S. Banger, and S. P. Singh, Phys. Rev. B **38**, 7415 (1988).
[6]S. T. Chui, Phys. Rev. B **9**, 2097 (1974).
[7]Y. Nagawaka and A. D. B. Woods, Phys. Rev. Lett. **11**, 272 (1963).
[8]W. Weber, in *Superconductivity in d- and f-Band Metals*, edited by D. H. Douglass (Plenum, New York, 1976).
[9]A. O. E. Animalu, Phys. Rev. B **8**, 3555 (1973).
[10]K. Terakura, J. Phys. F **14**, 3255 (1984).
[11]R. Collela and B. W. Batterman, Phys. Rev. B **1**, 3913 (1970).
[12]A. D. B. Woods and S. H. Chen, Solid State Commun. **2**, 233 (1964).
[13]A. D. B. Woods, Phys. Rev. **136**, A781 (1964).

[14]V. J. Minkiewiecz, G. Shirane, and R. Nathans, Phys. Rev. **162**, 528 (1967).
[15]J. M. Wills and W. A. Harrison, Phys. Rev. B **28**, 4363 (1983).
[16]W. B. Pearson, *A Handbook of Lattice Spacings and Structure of Metals and Alloys* (Pergamon, New York, 1958).
[17]M. W. Finnis and J. E. Sinclair, Philos. Mag. A **50**, 45 (1984).
[18]D. Lagersie and G. Allan, in *Lattice Dynamics,* edited by M. Balkanski (Flammarion, Paris, 1978).