Three-particle forces in hexagonal-close-packed Ho

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Clark-Gazis-Wallis-type three-particle forces are applied for the first time systematically to the lattice dynamics of the hcp system. The model explains the ordering of dispersion branches along the ΓKM direction for hcp Ho.

The Clark-Gazis-Wallis (CGW) angular force model,[1] involving three-particle forces, has been extensively applied in the study of the vibrational behavior of cubic metals by restricting the interatomic forces up to the second set of nearest neighbors.[2] In order to compare the major force-constant models and to resolve certain controversies, Moore and Upadhyaya[3] have done a systematic analysis to consider the CGW-type forces up to the third set of nearest neighbors in cubic systems. It is seen that the work of Yuen and Varshni[4] on a fcc system using the CGW model is not complete and even misleading because they do not consider the important set of 24 equilateral triangles made by the first nearest neighbors. The third-neighbor analysis is a little tedious and lengthy but results in the distinction between De Launary (two-body) and CGW (three-body) models for bcc and fcc structures. In the case of the hcp structure, CGW-type forces have been applied by a few workers only, perhaps due to the tedious and lengthy analysis involved in the application. Metzbower[5] was the first to apply the CGW model to the lattice dynamics of the hcp structure. In this work, the interaction between nearest neighbors in the basal plane were considered to be central while the interaction between both the nearest and next-nearest neighbors out of the basal plane were considered to be angular type. However, they have considered only the angles of the triangles connecting the reference atom to the two atoms out of the basal plane, leaving out other angles of the triangles. Further their analysis gives the $\mathrm{Im}D_{xy}^{11}$ element of the dynamical matrix to be zero and hence it cannot explain the ordering of the dispersion branches along the ΓKM direction and the degeneracy at the K point in the hcp metals such as Be, Tb, and Ho.[6] In further work, Kushwaha *et al.*[7] consider two types of triangles: type-I triangles are formed by joining the reference atom to two of its six neighbors in the basal plane, and type-II triangles are made by joining the reference atom to one atom in the basal plane and another atom in the $z=\pm c/2$ plane. This involves six equilateral triangles and 36 right-angled triangles. Their analysis involves two angular force constants, and hence it clearly shows that they do not consider the force constants corresponding to the acute angles of the right-angled triangles. Further, they also leave out the important sets of triangles made by the origin atom and its first and second nearest neighbors. In their analysis, although they get the $\mathrm{Im}D_{xy}^{11}$ element to be nonzero, they are not able to explain the peculiar behavior of the dispersion branches of the ΓKM direction in Be.

In the present work we apply the CGW model systematically for the first time to investigate the dynamical behavior of the hcp lattice. Here we consider three sets of triangles.

(1) Six equilateral triangles made by the origin atom and two of its nearest neighbors in the basal plane with sides a,a,a, and one angular force constant $\gamma_1(a,a)$.

(2) Six isosceles triangles, made by the reference atom and two nearest neighbors out of the basal plane of sides a,a',a $(a'^2=a^2/3+c^2/4)$ with angular force constants $\gamma_2(a,a')$ and $\gamma_3(a',a')$.

(3) Twelve isosceles triangles, made by the reference atom, one nearest-neighbor atom in the basal plane, and one nearest neighbor out of the basal plane of sides a,a',a' with angular force constants $\gamma_2(a,a')$ and $\gamma_3(a',a')$.

Thus, this analysis includes all triangles made by first and second sets of nearest neighbors with the maximum length a of a side for elements such as Be, Tb, and Ho. The dynamical matrix element $\mathrm{Im}D_{xy}^{11}$ is found to be

$$\mathrm{Im}D_{xy}^{11}=\sqrt{3}\left\{\left[\gamma_2\frac{1}{a^{14}}\left[\frac{c^2}{3}+\frac{a^2}{9}\right]+\gamma_3\frac{1}{a^{18}}\left[\frac{a^6}{18}+\frac{a^4c^2}{6}\right]\right]\sin\left(\tfrac{1}{2}aq_1\right)\cos\left[\frac{\sqrt{3}}{2}aq_2\right]\right.$$

$$\left.-\left[\gamma_2\frac{1}{a^{14}}\left[c^2+\frac{a^2}{3}\right]+\gamma_3\frac{1}{a^{18}}\left[\frac{a^4c^2}{12}+\frac{a^6}{36}\right]\right]\sin(aq_1)\right\},$$

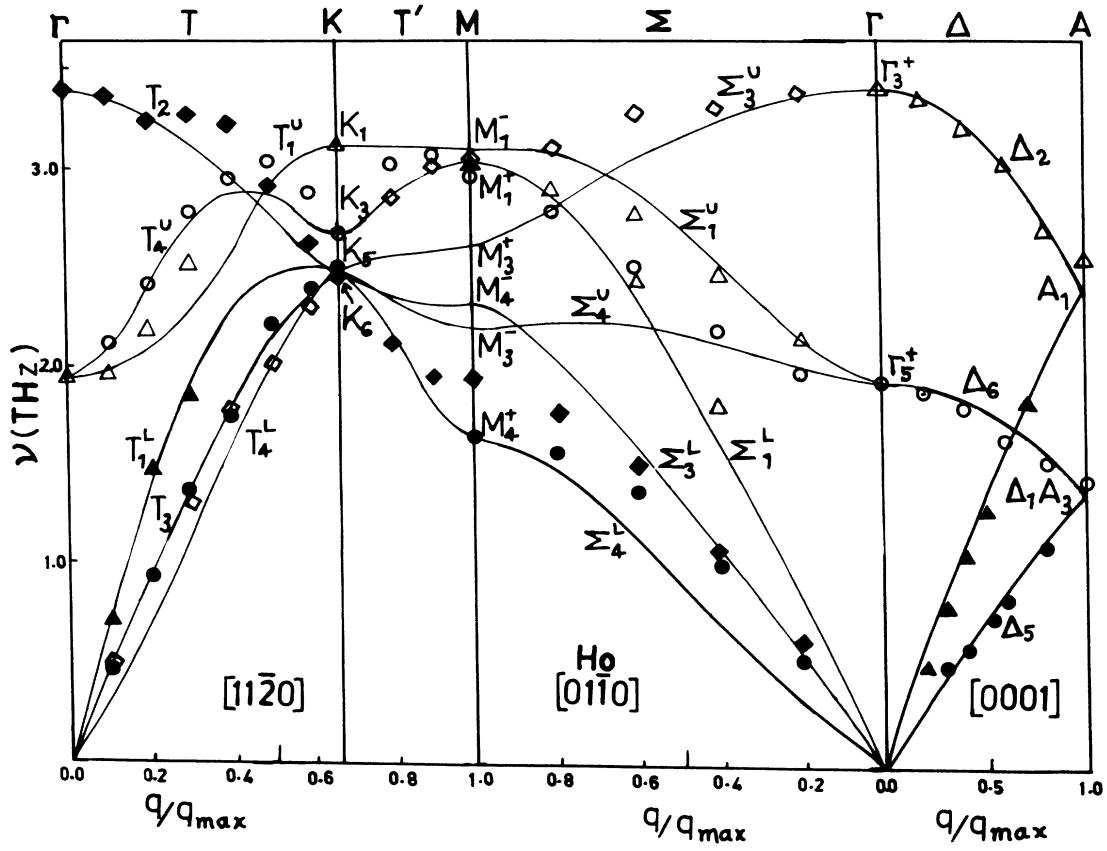

FIG. 1. Phonon dispersion in Ho: Solid curves represent the results of present calculations; ○, ●, △, ▲, □, ■: experimental points of Houmann and Nicklow (Ref. 10).

where, the wave vector $\mathbf{q}=q_1\hat{\mathbf{x}}+q_2\hat{\mathbf{y}}+q_3\hat{\mathbf{z}}$.

In view of the first-principles work of Bertoni *et al.*[8] on hcp Be, three-particle forces are known to be of short-range character. The analysis involves double sums on reciprocal-lattice vectors and hence involves much computer time. However, they have suggested the use of three-particle forces for a real-space analysis. That is why we have considered three-particle CGW interactions only up to the second set of nearest neighbors in the hcp system. The mathematical development of the CGW-type interaction in the hcp system was announced earlier.[9] We consider central interactions up to fifth nearest neighbors involving five force constants β_1, β_2, β_3, β_4, and β_5. The force parameters β_1, β_2, β_3, β_5, γ_1, γ_2, and γ_3 of the model are fixed from the known frequency expressions for $\nu(K_1)$, $\nu(K_3)$, $\nu(K_5)$, $\nu(\Gamma_3^+)$, $\nu(\Gamma_5^+)$, $\nu(M_1^+)$, and $\nu(M_4^+)$. We have omitted the β_4 parameter as it does not affect the dispersion branches in the ΓKM direction. The model parameters of hcp Ho used to compute the phonon frequencies in the present calculation are (in dyn/cm)

$$\beta_1=9445.481\,327,\quad \beta_2=-134.764\,054,$$

$$\beta_3=3688.742\,514,\quad \beta_5=-1420.825\,604,$$

$$\gamma_1=-969.857\,564,\quad \gamma_2=2190.990\,054,$$

$$\gamma_3=5704.471\,540.$$

Now, the secular equation

$$|D(\mathbf{q})-M\omega^2 I|=0$$

is solved to obtain the normal-mode phonon frequencies along the ΓA, ΓM, and ΓKM symmetry directions. Here $D(\mathbf{q})$ is the dynamical matrix, M the ionic mass, and I the unit matrix. Results of the calculation for Ho are presented in Fig. 1 and compared with the experimental data of Houmann and Nicklow.[10] We observe that the present model gives the correct ordering of the dispersion branches along the ΓKM direction and the desired degeneracy of T_1^L and T_4^L branches at the K point.

Thus, in the present work we apply for the first time systematically the CGW angular force model to the lattice dynamics of the hcp system. We have succeeded in explaining the peculiar behavior of the dispersion branches along the ΓKM direction. This behavior could not be explained by earlier workers who applied the CGW model to the lattice dynamics of the hcp system. Dispersion results in Be and Tb are also found to be similar and in reasonable agreement with the experimental data.

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