CHAPTER 5

PHONON FREQUENCIES OF PARAMAGNETIC hep TRANSITION METALS, SCANDIUM AND YTTRIUM

In chapters 2, 3 and 4, we studied the dielectric screening and the phonon dispersion relations of the bcc and fcc transition metals in the non-interacting band model scheme. In this chapter, the non-interacting band model scheme is extended to the hep transition metals and is applied to study the effect of the d-electrons in the dielectric screening and the phonon frequencies of scandium and yttrium which belong to the 3d and 4d series of the transition metals. The plan of this chapter is as follows: A brief account of the hep structure and the Brillouin zone is given in section 5.1. The non-interacting band models and the dielectric functions for scandium and yttrium are presented in sections 5.2 and 5.3, respectively. In section 5.4, the calculations of the phonon dispersion relations are presented. In last section 5.5, the results are concluded.

5.1 hep STRUCTURE AND BRILLOUIN ZONE

The hep structure consists of two interpenetrating simple hexagonal lattices and can be regarded as a Bravais lattice with a basis. If c is the distance between the two alternate planes and a is the distance between nearest neighbours in any plane, the hexagonal lattice vectors are defined as:

$$a_1 = a \hat{1} \ , \ a_2 = -(1/2) a \hat{1} + (\sqrt{3}/2) a \hat{2} \ , \ a_3 = c \hat{3} \ (5.1)$$
where $\mathbf{a}_1$, $\mathbf{a}_2$, and $\mathbf{a}_3$ denote the unit vectors along the cartesian axes. The unit cell of the hcp structure along with the direct lattice vectors $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$ and the primitive reciprocal lattice vectors $\mathbf{b}_1$, $\mathbf{b}_2$, $\mathbf{b}_3$ is shown in Fig. 5.1. The hcp structure has the space group $D_{6h}^1$ and the unit cell contains two atoms, one at the origin and the other at $(1/3) \mathbf{a}_1 + (2/3) \mathbf{a}_2 + (1/2) \mathbf{a}_3$. The volume of the unit cell is given as:

$$V = (\sqrt{3}/2) \ a^2 \ c,$$

and the atomic volume $\Omega_0$ is half of the unit cell volume $\Omega$. The reciprocal lattice vector $\mathbf{G}$ may be expressed as

$$\mathbf{G} = (2\pi/a) \ h_1 \ \mathbf{a}_1 + (2\pi/\sqrt{3}a) (h_1 + 2h_2) \ \mathbf{a}_2 + (2\pi/c) \ h_3 \ \mathbf{a}_3,$$

where $h_1$, $h_2$ and $h_3$ are all integers. The Brillouin zone of the hcp structure along with three principal symmetry directions $\Gamma K$, $\Gamma M$ and $\Gamma A$ is also shown in the Fig. 5.1. The volume of the Brillouin zone $\Omega_B$ is related to the unit cell volume by the relation

$$\Omega_B = 8\pi^3 / \Omega.$$

### 5.2 NON-INTERACTING BAND MODEL FOR SCANDIUM AND YTTRIUM

In this section we construct the isotropic non-interacting band models for scandium and yttrium. These metals are the simplest hcp transition metals and are chosen for the following reasons:

The experimental data for the phonon dispersion relations are...
available and these are free from magnetic ordering effects, unlike rare earth metals. The phonon dispersion relations are also similar to those of simple hcp metals such as beryllium and magnesium though their electronic band structures are entirely different. The anisotropy in these metals is also expected to be small because the c/a ratios are near to the ideal value. The band structure calculations and the other required informations are also available for these metals.

The data for the band structure of the hcp transition metals are rare with the exception of cobalt which is ferromagnetic. Altmann et al. and Loucks have carried out the band structure calculations for scandium and yttrium but these authors do not tabulate the energy eigenvalues. However, we use the calculations due to Altmann et al. to construct the non-interacting d-band model by reproducing the energy eigenvalues from the enlarged graphs. The bands show s- or p- character at the centre of the Brillouin zone but towards the zone boundary the d-character dominates. In order to simplify the construction of the non-interacting band model we consider only those bands which are either below or intersect the Fermi energy because the electrons only in these bands have a dominating role in the dynamical properties. For scandium, the non-interacting band model, along the principal symmetry directions $\Gamma K$, $\Gamma N$ and $\Gamma A$, is shown by the solid lines in Fig. 5.2. The d-sub bands are joined according to the compatibility relations of the hcp structure. Along the $\Gamma M$ direction the point $\Lambda_1$ is
compatible with both the points $A'$ and $A''$ and therefore the band from $A'_1$ is joined to the lower symmetry point $A'_1$. In the symmetry direction $P'A$, one d-sub band is completely filled but the other two d-sub bands are completely empty. Along the $\Gamma K$ direction all the three d-sub bands are partially filled. The d-sub bands along all the three symmetry directions are labelled as 1, 2 and 3.

Similar procedure is adopted to construct the non-interacting band model for yttrium using the results for the band structure calculations of Altmann et al. and is shown in Fig. 5.3. In the $\Gamma K$ direction all the three d-sub bands are partially filled and are joined according to the compatibility relations. In the $\Gamma M$ direction, one d-sub band is completely filled, one is partially filled and the third is completely empty. In the $P'A$ direction one d-sub band is completely filled and the other two d-sub bands are completely empty. It is evident from the Figs. 5.2 and 5.3 that the non-interacting d-sub bands for scandium and yttrium are similar to each other and both are similar to those obtained by Mori et al. for hcp cobalt in the tight-binding limit.

The atomic configurations for scandium and yttrium are $(3d)^{12} (4s)^2$ and $(4d)^1(5s)^2$, respectively. But these configurations are not consistent with the other calculations and the experimental observations for these metals. Loucks has shown, in yttrium, that the electronic specific heat, which is directly related to the density of states, is
increased three times than the free electron value if the effect of the d-electrons is considered. The same conclusion is also drawn by Dimmock and Freeman\textsuperscript{69} for gadolinium which has similar energy bands as those for yttrium. Therefore, it is concluded that the d-electrons must be twice in number than the s-electrons which suggests the electronic configuration \((4d)^2(5s)^1\) for yttrium in the metallic phase. Since scandium and yttrium belong to the same group and have similar band structures, therefore, the electronic configuration \((3d)^2(4s)^1\) is chosen for scandium. The above configurations are also supported by the Knight shift study of transition metals due to Jaccarino.\textsuperscript{127}

The calculation of the dielectric matrix along the different symmetry directions separately, is very difficult from the computational point of view. To simplify the calculations and to study the effect of the d-electrons in the lattice dynamics of hcp transition metals we construct an isotropic non-interacting energy band model as we did for bcc and fcc transition metals. From the non-interacting band model we first calculate the occupied volume of the d-sub bands labelled as 1, 2 and 3 along the three principal symmetry directions \(\Gamma K, \Gamma M\) and \(\Gamma A\) and completely ignore the empty d-sub bands which are far away from the Fermi surface and which hardly affect the dynamical properties. Then we take the simple average of the occupied volume of the d-sub bands considering only those symmetry directions along which the d-sub bands are filled or partially filled. The two d-electrons are distributed
among the d-sub bands in the ratio of the average volume occupied by
them. The Fermi momenta for the d-sub bands and the s-band are calculated
in the parabolic band approximation given by Eqs. (2.53) and (2.54),
respectively. The effective masses for the d-sub bands are calculated
in the same way as done by Prakash and Joshi by replacing the
Brillouin zone by a sphere of radius $r_B$, except that equal weightage is
given to all the three principal symmetry directions in averaging the
energy eigenvalues at the Brillouin zone boundary and only those d-sub
bands are considered which are filled or partially filled. The isotropic
band models, constructed in this manner are shown in Figs. 5.4 and 5.5
for scandium and yttrium, respectively. The d bond-widths for scandium
and yttrium, in our isotropic band models, are 0.27 and 0.24 ryd.,
respectively, which are 13% and 20% less than the average d bond-widths
calculated from the actual calculations of Altmann et al. Therefore,
in the hop transition metals too we treat the d-electrons more tightly
bound to the core than in the detailed band structure calculations. The
physical parameters, the charge distribution, effective masses and
the Fermi momenta for all the s-and d-sub bands are given in the Table
5.1 for both the metals. The assignment of the magnetic quantum number
is not needed in the present calculations because all the active d-
sub bands considered here are non-degenerate and only the compatibility
relations resolve the difficulties.
5.3 DIELECTRIC MATRIX

From the isotropic non-interacting band models shown in the Figs. 5.4 and 5.5 it is evident that all sorts of intraband and interband transitions, as described in chapter 2 for paramagnetic chromium are also allowed for both the metals scandium and yttrium. To calculate these contributions to the dielectric matrix the Eqs. (2.19), (2.24), (2.25), (2.38), (2.41), (2.44), (2.45), (2.51) and (2.52) are used in the same way as in the bcc and fcc transition metals. The 3d radial wavefunction for scandium is taken from the calculations of Clementi\textsuperscript{91} represented in the analytical form given by Eq. (2.36). The 4d radial wavefunction for yttrium is not available in the parameterized form from the calculations of Clementi, therefore, we have taken it from the calculations of Herman and Skillman\textsuperscript{117} and represented it in the analytical form given by Eq. (2.36) by the least square fit method within the accuracy of ±1%. The parameters $a_1$ and $\alpha_1$ for both the metals are tabulated in the Table 5.2.

The hybridization between the $m$ components of the d-wavefunction for a particular d-sub band is taken by averaging over all the $m$ components as done in the bcc and fcc metals. The qualitative behaviour of the diagonal contribution of the dielectric matrix is found to be the same as in paramagnetic bcc and fcc transition metals. The contribution of the nondiagonal terms is again estimated in the same way as done for the bcc and fcc metals. In scandium, the local
field corrections due to both the intraband and the interband transitions are found to be negative. But in yttrium, the local field corrections due to the intraband transitions are positive but those due to the interband transitions are negative. Sinha et al. found the local field corrections to be negative for silicon. Such a behaviour is also found by Vechton and Martin for diamond and by Czachor for semimetals in a two band model.

5.4 PHONON DISPERSION RELATIONS

In the isotropic non-interacting band models for scandium and yttrium the s-band and all the three d-sub bands are partially filled. Therefore, for scandium and yttrium the ion cores are limited to (3p) and (4p), respectively, and there are three conduction electrons per atom in both the metals. The Coulomb coupling coefficients between the ions are calculated using the Eq. (3.51) and these are tabulated in Tables 5.3 and 5.4 for a selected set of phonon wave-vectors for scandium and yttrium, respectively, and which may be useful for future calculations. The core-core exchange overlap interaction contribution is neglected because of the small core size.

In the evaluation of the ion-electron-ion coupling coefficients the functions $B(q+G)$ and $F(q)$, introduced in Eqs. (3.15) and (3.16), for both scandium and yttrium are represented in the analytical form given as:

$$B(q+G) = \alpha_7 |q+G|^2 \exp[\alpha_8 |q+G|^2]$$

for $|q+G| \ll P_1$.
\[ w \propto 1 \left| q+G \right|^2 \exp\left\{ -\alpha_2 \left| q+G \right|^\alpha_3 \left| q+G \right|^2 \right\} \]

for \( p_1 \ll \left| q+G \right| \ll p_2 \)

\[ = \alpha_4 \exp\left\{ -\alpha_5 \left| q+G \right|^2 \right\} \]

for \( \left| q+G \right| \gg p_2 \), \( (5.5) \)

and

\[ F(q) = -\alpha_6 \frac{m}{s} \frac{k_F}{s} \left\{ 1 + \frac{4k^2_{F,s} - q^2}{4k_{F,s} q} \ln \left| \frac{2k_{F,s} + q}{2k_{F,s} - q} \right| \right\} \]

\( (5.6) \)

Here the parameters \( \alpha_1, \alpha_2, \alpha_3, \alpha_4, \alpha_5, \alpha_6, \alpha_7, \alpha_8 \), \( p_1 \) and \( p_2 \) are obtained by fitting the actual interband contribution within \( \pm 10\% \) and these parameters are tabulated in Table 5.5 for both the metals. We replace the bare ion potential by the renormalized Animalu TMIP which was also used in our earlier calculations of the phonon frequencies of the hcp metals \( ^{66} \) and in other transition metals \( ^{56-58} \) and which yielded a reasonable agreement with the experimental values. The exchange and correlation corrections are applied to the s- and the d-electrons separately in the same manner as described in case of the bcc and fcc metals in earlier chapters. Lindgren et al. \(^{74} \) have not done the calculations for \( a' \) of the 4d shell. Therefore in the absence of the detailed calculations we use the same value of \( a' \) for yttrium and scandium as they belong to the same group in the periodic table and have similar electronic configurations. A similar procedure was also adopted for palladium and platinum. The parameter \( a' \) for both the metals scandium and yttrium is also given in the Table 5.5.
The phonon frequencies are calculated along the principal symmetry directions [0001] and [0110] using the expressions given below, obtained by Czachor \(^6\) by factorizing the secular equation,

(a) [0001] direction, z polarization, longitudinal mode:

\[
\omega^2 (q_z) = D_{zz} (q_{jj}) \pm |D_{zz} (q_{jj'})| ,
\]

\[
(q_x = q_y = 0; q_z = q_z) .
\] (5.6a)

(b) [0001] direction, x or y polarization, transverse modes:

\[
\omega^2 (q_z) = D_{xx} (q_{jj}) \pm |D_{xx} (q_{jj'})| ,
\]

\[
(q_x = q_y = 0; q_z = q_z) .
\] (5.6b)

(c) [0110] direction, y polarization, longitudinal mode:

\[
\omega^2 (q_y) = D_{yy} (q_{jj}) \pm |D_{yy} (q_{jj'})| ,
\]

\[
(q_x = q_z = 0; q_y = q_y) .
\] (5.7a)

(d) [0110] direction, x polarization, transverse mode \(\|\) to basal plane:

\[
\omega^2 (q_y) = D_{xx} (q_{jj}) \pm |D_{xx} (q_{jj'})| ,
\]

\[
(q_x = q_z = 0; q_y = q_y) .
\] (5.7b)

(e) [0110] direction, z polarization, transverse mode \(\perp\) to basal plane:

\[
\omega^2 (q_y) = D_{zz} (q_{jj}) \pm |D_{zz} (q_{jj'})| ,
\]

\[
(q_x = q_z = 0; q_y = q_y) .
\] (5.7c)

The plus sign is for the optical modes and the minus sign is for the
acoustic nodes. The expressions for $D_{ij'}^{\alpha\beta}$ for a lattice with
basis are given by the Eqs. (3.43), (3.48), (3.51) and (3.55).

The Anatomu TNP is renormalized in the same way as we did in
our earlier calculations of the phonon frequencies for the hop metals.
The parameter $\lambda_0^2$, which represents the hybridisation, is retained to be
the same and the parameters $\lambda_0$ and $R_m$ are renormalized by matching the
phonon frequencies in the longitudinal branch in the [0001] direction
at the symmetry point $A$ for both the metals. The renormalized parameters
are given in Table 5.6. The phonon dispersion relations for scandium
and yttrium are shown in Figs. 5.6 and 5.7, respectively, with solid
lines. The experimental results of W&kabayashi et al.\textsuperscript{123} for scandium
and Sinha et al.\textsuperscript{122} for yttrium are also shown there. For comparison the
results obtained by using the parameters tabulated by Ananlu\textsuperscript{55} in
conjunction with the free electron dielectric function are also shown in
the Figs. 5.6 and 5.7 with dashed lines.

For scandium in the [0001] direction, the LA and the TA
branches are in good agreement with the experimental values. The LO
and TO branches, in the [0001] direction, show good agreement near the
zone boundary but the calculated phonon frequencies are lower than
the experimental values by about 5% in both the branches for the small
and the intermediate values of the wavevector. In the symmetry direc-
tion[010], the TA branch shows a close agreement with the exper-
imental values while the calculated phonon frequencies in all other
branches are lower than the experimental values with a maximum
deviation of about 13% near the zone boundary. In the experimental data the TO\perp, TO||, La and LO branches in the [01\bar{1}0] direction are nearly degenerate at the zone boundary. In our calculations La, LO and T0\perp branches are nearly degenerate but the TO|| branch is lower than the experimental values by about 13%. Again the experimental TA|| and TA\perp branches are nearly degenerate at small values of the phonon wavevector q while such a degeneracy is not found in our calculations. By comparing the results presented by the solid and the dashed lines it becomes evident from the Fig. 5.6 that the agreement with the experimental values in all the polarization branches is considerably improved by taking into account the effect of the partially localized d-electrons.

We find in our calculations of the phonon frequencies for scandium that the initial slopes of the longitudinal branches LA, in both the symmetry directions [0001] and [01\bar{1}0], are approximately the same which is consistent with the experimental observations. The transverse branches TA|| and TA\perp, in the [01\bar{1}0] symmetry direction, have approximately the same slope as the transverse branch TA in the [0001] direction in our calculations which is again consistent with the experimental results. Therefore, our calculation for the phonon dispersion relations also shows that there is considerable directional acoustic isotropy.

In the experimental data for scandium, the Kohn anomaly is found at \( q = (0,0,0.27) \frac{2\pi}{c} \) in the LA branch in the [0001] direction and it is very weak. It is assumed to arise due to the
nesting of the Fermi surface of scandium along the c-axis. But in our calculations we did not find such an anomaly. This may be due to the fact that we have used the spherical Fermi surfaces for the s- and d-electrons which may not exhibit the nesting of the Fermi surface.

For yttrium the calculated phonon frequencies in the LA and TA branches in the [0001] direction are in good agreement with the experimental values. The calculated phonon frequencies of the LO and TO branches, in the [0001] direction, are in good agreement with the experimental values near the zone boundary but are higher by about 4.5% in the LO branch and are lower by about the same magnitude in the TO branch near the centre of the Brillouin zone. In the [0110] direction, the calculated phonon frequencies in the TA1 branch are higher than the experimental values by about 15% near the zone boundary. All the other branches in the [0110] direction are lower than the experimental values with a maximum deviation of about 9% near the zone boundary. Again, the TA11 and TA1 branches are found to be nearly degenerate experimentally at small values of q; but such a degeneracy is not found in our calculations. In yttrium also all the polarization branches are improved over the simple metal-like calculations.

The acoustic isotropy is also found in the phonon dispersion relations of yttrium which is consistent with the experimental observations of Sinha et al. In yttrium, two anomalies are found experimentally in the double Brillouin zone scheme at \( q = (0.0,0.0,0.625) \times 2\pi/c \) and \( (0.0,0.0,0.775) 2\pi/c \). We have not investigated...
these anomalies as we restrict our calculations of the phonon frequencies in the first Brillouin zone.

For both the metals, it is found that in the longitudinal branches the diagonal and the nondiagonal contributions sum up to a maximum of 2% but in the transverse branches the diagonal and the nondiagonal contributions cancel each other and therefore the transverse branches are not renormalized by the d-type contribution. Therefore in hep metals also the local field corrections behave in the same way as in bcc and fcc metals.

5.5 CONCLUSIONS

The electronic band structure of the hcp transition metals is much more complicated as compared to that of the bcc and fcc transition metals. The problem of constructing a non-interacting band model is simplified by considering only those bands which are filled or partially filled and it is justified because the electrons only in these bands give the major contribution to the dynamical properties of the metals. However, ours is the first attempt to study the effect of the d-electrons on the phonon dispersion relations of a low symmetry hep structure and it is found that the results for the phonon dispersion relations are improved which becomes evident by comparing the calculations with the free electron like calculations. The contribution of the local field corrections is appreciable towards the phonon frequencies of the hcp metals. The general features of the phonon frequencies are found to be the same as that of the experimental values inspite of the various approximations used in constructing the non-interacting band model.
### TABLE 5.1.A Physical parameters for scandium (atomic units).

<table>
<thead>
<tr>
<th>Lattice constants</th>
<th>a=6.2552, c=9.9584</th>
</tr>
</thead>
<tbody>
<tr>
<td>c/a</td>
<td>1.5920</td>
</tr>
</tbody>
</table>

Atomic volume \( V_0 = 168.7 \times 10^3 \)

Radius of the Brillouin sphere \( r_B = 0.8070 \)

Effective masses, Fermi momenta and charge distribution for the s- and d-sub bands (atomic units).

#### s-band

<table>
<thead>
<tr>
<th>( k_{Fs} )</th>
<th>( m_s )</th>
<th>( Z_s )</th>
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<tr>
<td>0.5599</td>
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#### d-sub bands

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<th>( m_{d1} )</th>
<th>( Z_{d1} )</th>
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<tr>
<td>1</td>
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<td>1.1563</td>
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<td>2</td>
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<td>3</td>
<td>0.2727</td>
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### TABLE 5.1.B Physical parameters for yttrium (atomic units).

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</thead>
<tbody>
<tr>
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</tbody>
</table>

Atomic volume \( V_0 = 223.1 \times 10^3 \)

Radius of the Brillouin sphere \( r_B = 0.7360 \)

Effective masses, Fermi momenta and charge distribution for the s- and d-sub bands (atomic units).

#### s-band

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<th>( k_{Fs} )</th>
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(contd.....next page)
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<th>( Z_{di} )</th>
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TABLE 5.2 Parameters for the 3d and 4d radial wavefunctions for scandium and yttrium.

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<tr>
<th></th>
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<th>Y (a_i)</th>
<th>Y (α_i)</th>
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<tr>
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<td>5</td>
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<td>1.0000</td>
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<td>—</td>
</tr>
<tr>
<td>Direction</td>
<td>Re D(x,x)</td>
<td>Im D(x,x)</td>
<td>Re D(y,y)</td>
<td>Im D(y,y)</td>
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<td>-----------</td>
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</tr>
<tr>
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<td></td>
<td></td>
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<tr>
<td>zz</td>
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<td></td>
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</tbody>
</table>

**TABLE 5.3 Coulomb coupling coefficients for scandium**

*Units of D(x,x) in eV*
TABLE 5.4 Coulomb coupling coefficients for yttrium lines of (4f^2 e /M *l^2). In units of (4f^2 e /M *l^2).
TABLE 5.5 Parameters of the interband part of the dielectric matrix and exchange correlation corrections for scandium and yttrium.

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<thead>
<tr>
<th>Parameters</th>
<th>Scandium</th>
<th>Yttrium</th>
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<tbody>
<tr>
<td>$\alpha_1$</td>
<td>44.0900</td>
<td>184.4000</td>
</tr>
<tr>
<td>$\alpha_2$</td>
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<tr>
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<tr>
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<td>$\alpha_8$</td>
<td>1.0000</td>
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</tr>
<tr>
<td>$p_1$</td>
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</tr>
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</tr>
<tr>
<td>$\alpha'$</td>
<td>0.4900</td>
<td>0.4900</td>
</tr>
</tbody>
</table>
TABLE 5.6 Parameters of the renormalized Animalu fMMP for scandium and yttrium. All the parameters are in atomic units except $|E_c|$ which is in ryd.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Scandium</th>
<th>Yttrium</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_0$</td>
<td>1.300</td>
<td>0.950</td>
</tr>
<tr>
<td>$A_1$</td>
<td>1.650</td>
<td>1.300</td>
</tr>
<tr>
<td>$A_2$</td>
<td>1.400</td>
<td>1.100</td>
</tr>
<tr>
<td>$R_m$</td>
<td>1.600</td>
<td>1.750</td>
</tr>
<tr>
<td>$Z$</td>
<td>3.000</td>
<td>3.000</td>
</tr>
<tr>
<td>$R_c$</td>
<td>1.531</td>
<td>1.739</td>
</tr>
<tr>
<td>$\alpha_{\text{eff}}$</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>$</td>
<td>E_c</td>
<td>$</td>
</tr>
</tbody>
</table>
FIGURE CAPTIONS

Fig. 5.1 Unit cell and Brillouin zone for hop structure. \( \mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3 \) are the primitive vectors of the direct lattice and \( \mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3 \) are the primitive vectors of the reciprocal lattice.

Fig. 5.2 Non-interacting band model for scandium along the principal symmetry directions \( \Gamma K, \Gamma M \) and \( \Gamma A \). The dashed line shows the Fermi energy. The dash-dot lines show the band structure due to Altmann et al. [Ref. 67]. The d-sub bands are numbered as 1, 2 and 3.

Fig. 5.3 Non-interacting band model for yttrium along the three principal symmetry directions \( \Gamma K, \Gamma M \) and \( \Gamma A \). The description is the same as that of Fig. 5.2.

Fig. 5.4 Isotropic non-interacting band model for scandium. The dashed line shows the Fermi energy. The d-sub bands are numbered as 1, 2 and 3.

Fig. 5.5 Isotropic non-interacting band model for yttrium. The description is the same as that of Fig. 5.4.

Fig. 5.6 The phonon dispersion relations for scandium. The solid lines represent the present calculations and the dashed lines represent the results using the parameters tabulated by Animalu [Ref. 55] and the free electron dielectric function. The experimental results are due to Wakabayashi et al. [Ref. 123].

Fig. 5.7 The phonon dispersion relations for yttrium. The description is the same as that of the Fig. 5.6. The experimental results are due to Sinha et al. [Ref. 122].
FIG. 5.4
FIG. 5.5

ENERGY (RY)

0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0

A_{2+}^*
A_{1-}^-
A_{1+}^-
E_-
S-BAND

FERMI ENERGY

k (a.u.)

0.0
0.2
0.4
0.6

FIG. 5.5