SIMPLIFIED FORMS OF THE FIELEK MODEL FOR bcc TRANSITION METALS

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Two simple forms of the FIELEK [1] model are developed to infer about the nature of the interactions among neighbouring d-shells, characterising the transition metals. The first model expresses this interaction as the sum of first two terms of the Taylor’s expansion for energy, while the second model describes this interaction to be three body (angular or unpaired) type. Both of these models obey the equilibrium condition and represent core-core interactions to be central pairwise extending to immediate neighbours only. Volume interactions among core and conduction electrons and also among d-shells and conduction electrons follow the modified BHATIA Scheme [5].

The theoretical findings given by these models on phonon dispersion in bcc zirconium and niobium are compared with the experimental data. Further these findings are also compared with those of the original FIELEK model which is simplified by substituting the said BHATIA scheme for that due to KREBS [3].

Introduction

Passage of thermal wave through lattice causes changes in coupling energy of the various constituents of a transition metal. According to FIELEK [1] this change is expressed as a sum of the second order changes in the potential energy coupling the constituents. First order changes, which are responsible for inequality [2] between the statical and dynamical elastic constants, are completely ignored while developing the FIELEK model. Moreover, this omission leaves the crystal in a state of inequilibrium. The FIELEK model [1] assumes the second order changes in the coupling energy of the system comprising core and conduction electrons to be negligibly small. This drawback poses difficulties regarding the cohesion and the stability of the lattice. Further the FIELEK Model [1] describes the volume interactions among d-shells and conduction electrons on the lines of KREBS scheme [3] which (a) depicts the perfectly free picture of the electron gas, (b) does not include the condition for crystal equilibrium and (c) involves enormous computational efforts.

Presently we have developed two different models. The first model expresses the core—core and the d shell — d shell interactions separately as the

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sum of first and second term of the respective Taylor's expansions. In our
second model the core—core interactions remain the same but the mutual inter-
actions among the d-shells are considered to be unpaired and described within
the framework of the angular scheme due to Clark et al [4].

The effect of core—d shell energy in both models is considered on the
lines of the Fielek model. The volume interactions are included on the lines
of Bhatia [5] scheme which is modified (a) to incorporate the crystal aniso-
tropy by using an inference factor $C^2$ which distributes the total force over
the polyhedron-shaped atomic cell as a whole and (b) to account for the exchange
and correlation effects associated with the conduction electrons by employing
a proper dielectric function ($q$). Equilibrium conditions for both models are
derived in a physically consistent and simple manner. The Fielek model
is thus made physically sound and computationally less intricate as far as the
description of the equilibrium condition [6] and the volume interactions are
concerned.

The two models are employed to derive the dispersion relations in bcc
zirconium and niobium. To show the relative merits of the model, the results
on phonon dispersion are compared (a) with the experimental data on the
said metals and (b) with the theoretical findings of the original Fielek model,
which is simplified by using the said Bhatia scheme to take care of the volume
interactions.

Theory

The frequencies ($v$) of the normal modes are obtained by solving the
following secular determinant

$$| D(q) - 4\pi^2 \nu^2 I | = 0 ,$$

where $m$ is the mass of the core and $I$ is the unit matrix of the order three.
The elements of the dynamical matrix $D(q)$ may be written in terms of the
first ($\alpha_1$) and the second ($\beta_1$) derivatives of the central pairwise energy coupling
the immediate neighbours, i.e.

$$D_{\alpha\alpha}(q) = - \frac{8}{3} (\beta_1 + 2\alpha_1)(1 - C\alpha C\beta C\gamma) + K + AG_{\alpha\alpha}(q) + \frac{K^2}{N} ,$$

$$D_{\alpha\beta}(q) = - \frac{8}{3} (\beta_1 - \alpha_1) S\alpha S\beta C\gamma ,$$

where $S\alpha = \sin (1/2 aq\alpha)$, and $C\alpha = \cos (1/2 aq\alpha)$, $a$ is the lattice constant and $q\alpha$
is the $\alpha$-component of the phonon wave vector ($q$). $K$ is a parameter appearing
due to the interaction among the cores and the $d$-shells. The term $N$ is evaluated.