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Phonon anomalies in HfN

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Abstract
The phonon dispersion curve are determined by model (BSM) for the crystals transition metal mono-nitride (HfN) and compared with the experimental phonons, which forms perhaps the best test for this purpose. The eight numbers of parameters of the model are determined by using the some set of input data. The results and degrees of agreement obtained in each case show clearly the superiority of the "charge-transfer mechanism" for representing the deformations of electron shells used in the BSM. The phonon dispersion curves and phonon density of states in HfN have been measured in high-symmetry directions Δ, Σ and Λ by breathing shell model (BSM). Anomalies in the dispersion of the acoustic branches and optical branches have been detected which are well described by experimental results.

Keywords: Lattice dynamics, phonons in crystal lattices, thermal properties of crystalline solids, phonon states and phonon dispersion ,PACS no: 63, 63.20.-e, 65.40.-b, 63.20. Dj.

INTRODUCTION

Besides a number of exciting physical properties, transition metal (TM) nitrides compounds adopt several crystal structures, crystal lattices and form different phases depending on the R_x/R_M ratio where R_M and R_x are the atomic radii of metallic and non-metallic atoms, respectively. Almost all the nitrides of TM are usually cubic, where the metallic atoms form the face-centered cubic (fcc) sub lattice and non-metallic atoms occupy interstitial positions, forming NaCl-type structure and for many of them, the phonon dispersion curves have been measured by coherent inelastic neutron scattering [1-10]. The general nature of the optic branches is for most of the TMN, similar to that of ionic compounds with the rock-salt structure. The longitudinal branches (LO) lie above the transverse branches (TO), due to the long-range Coulomb interactions that are screened by the conduction electrons. This metallic screening destroys the Lyddane-Sachs-Teller Splitting [11] and results in a degeneracy of the LO and TO modes at the center of the Brillouin zone. However for most of the TM compounds the screening vector is small compared to the dimensions of the Brillouin zone. The LO branches therefore recover quickly from the screening effect and are for most of the TMN found above the TO branches. The only exceptions are UC [3], UN [5] and as the results of the present measurements show HfN. The most successful model so far in reproducing the measured phonon dispersion curves of transition metal carbides and nitrides with rock salt structure is the breathing shell model [12]. We shall use breathing shell model (BSM) for the purpose of assessing the role played by the breathing motion of the valance electrons. Here we used this model theory to calculate complete phonon dispersion curve of transition metal mononitride (HfN) compound. In addition, the effect of anion and cation polarizabilities on the phonon spectrum is analysed by this theory. The anomalies in the dispersion of the acoustic branches and optical branches have been detected which are well described by experimental results.

Theory of Model Applied

The Breathing Shell Model (BSM) [12] is the isotropic deformation of spherical electron shells is considered in the form of expansion and /or contraction of these shells during lattice vibrations. Using the shell model notations of woods et.al. [13] and introducing these ideas in the theory of shell model, we get the basic equations of motion for BSM as follows:

$$D(q)=(R'+ZCZ)-(R'-ZCY)(R'+G+YCY)^{-1}(R'+YCZ) \quad (1)$$

where $R'= (R-QH^{-1}Q^{\dagger})$; C and R are the Coulomb and short-range repulsive interaction matrices respectively. Q is (6×2) matrix representing the interactions between the ion displacements and breathing mode variables. The H is a (2×2) matrix and represents the interactions between the breathing mode variables of different ions in the lattice. These breathing matrices Q and H are written as [12]

$$Q=\begin{bmatrix} 0 & D \\ D & 0 \end{bmatrix} \quad (2)$$

The explicit expressions for these dynamical matrix.G and A are the diagonal matrices and represent the core-shell interaction and shell charge, respectively. The parameter involved in the dynamical matrix ***D(q)*** are determined by some microscopic experimental data, i.e. elastic constant, dielectric constant etc.. In order to minimize the number of parameters, we have assumed the shell charges, $Y_1=Y_2=Y$. The parameters are tabulated in the Tables.

RESULTS AND DISCUSSION

The phonon spectra obtained above have been used to predict the phonon dispersion relations $w_j(q)$ for HfN which are measured from inelastic neutron scattering. This BSM [12] has been used by jha and co worker [14, 15] to explain satisfactorily the anomalous phonon properties in rare earth chalcogenides and pnictides. The phonon dispersion relations along principal symmetry directions Δ, Σ and Λ, using a phenomenological model theory, which include the short-range breathing motion of the valance

electrons. For this purpose we derive the model parameters self consistently, using known macroscopic properties which include equilibrium lattice constant, elastic constants, zone center vibrational frequencies, ionic polarizabilities and dielectric constants. The input data used for this purpose are given in Table1. and also output parameters are listed in Table2. The phonon dispersion curve of HfN have been displayed in Fig.1. The measured data from this model are compared to the results of experimental inelastic neutron scattering values [8, 16]. ○ and ▲ represents the experimental points of longitudinal and transverse phonons respectively. The simple nature of the optic branches is for most of the TMC and TMN, similar to that of ionic compounds with the rock-salt structure. The longitudinal branches (LO) lie above the transverse branches (TO) due to the long-range coulomb interactions that are screened by the conduction electrons. In optic and acoustic branches are separated by an energy gap. It is revealed from Fig.1 that in case of HfN the theoretical results of PDC is in good agreement with experimental data along (q 0 0), (q q 0) and (q q q) directions for LO, TO and LA, TA modes. Because of the screening due to conduction electrons the LO and TO modes are degenerate at the **Γ** point, whereas the splitting of LO and TO modes at the **L** point is due to the long-range coulomb interaction which is not completely screened at larger **q** vectors. Strong electron-phonon interactions might be responsible for such peculiar behaviours.

Table 1. Input Parameters of HfN

Input Parameters	a_0 (Å)	C_{11} (Mbar)	C_{12} (Mbar)	C_{44} (Mbar)	$\nu_{TO}(\Gamma)$ THz	$\varepsilon_0 = \varepsilon_\infty$*	α_1 (Å^3)†	α_2 (Å^3)†
HfN	4.52[a]	6.79[b]	1.19[b]	1.50[b]	14.74[c]	3.60	0.162	1.10

[a][19], [b][17], *,† calculated values †[18], [c][16]

Table 2. Model Parameters for HfN. All are in units of $e^2/2V$ except Y in units of e.

Input Parameters	A_{12}	B_{12}	A_{11}	B_{11}	B_{22}	Z	$Y=Y_1=Y_2$	G_1	G_2
HfN	55.28	-1.17	30.46	-9.99	-17.86	1.68	2.78	2.26	1104.1

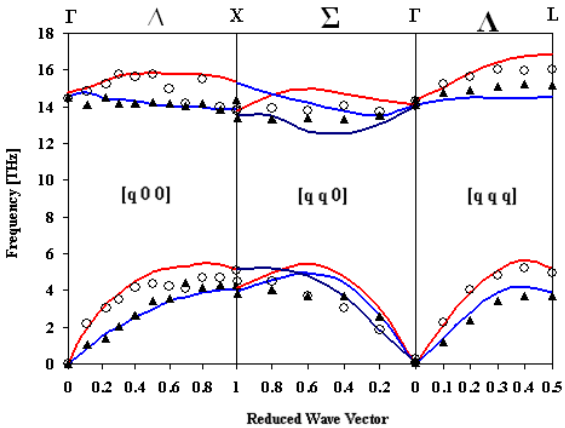

Fig 1. PDC from BSM fit for HfN, shows red, blue and black line; ○ and ▲ shows experimental [16] points of longitudinal and transverse phonons, respectively.

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