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DIRECT CORRELATION OF OBSERVED PHONON ANOMALIES AND
MAXIMA IN THE GENERALIZED SUSCEPTIBILITIES OF
TRANSITION METAL CARBIDES

By

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DIRECT CORRELATION OF OBSERVED PHONON ANOMALIES AND
MAXIMA IN THE GENERALIZED SUSCEPTIBILITIES OF
TRANSITION METAL CARBIDES*

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The generalized susceptibility, $\chi(\vec{q})$, of both NbC and TaC determined from APW energy band calculations show large maxima to occur at precisely those $\vec{q}_{\max}$ values at which soft phonon modes were observed by Smith. Maxima in $\chi(\vec{q})$ are predicted for other directions. The locus of these $\vec{q}_{\max}$ values can be represented by a warped cube of dimension $\sim 1.2 (\frac{2\pi}{a})$ in momentum space - in striking agreement with the soft mode surface proposed phenomenologically by Weber. In sharp contrast, the $\chi(\vec{q})$ calculated for both ZrC and HfC - for which no phonon anomalies have been observed - fall off in all symmetry directions away from the zone center. We thus interpret the phonon anomalies in the transition metal carbides as due to an "overscreening" effect resulting from an anomalous increase of the response function of the conduction electrons.

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I. Introduction

The phonon dispersion curves of the transition metal carbides (TMC) of the Metal IV and V series have been studied extensively by Smith and Gläser⁽¹⁾, and Smith⁽²⁾. These coherent inelastic neutron scattering experiments showed the important correlation that the high critical temperature (T_c) superconducting 9 valence electron compounds like NbC ($T_c = 11.1$ K) and TaC ($T_c = 10.35$ K) possess anomalies in their phonon spectrum which are not present in the low T_c ($T_c \leq 0.05$ K) 8 valence electrons compounds like ZrC and HfC. Such a correlation between phonon anomalies and high values of T_c has been also observed for a large number of d electron superconducting compounds or alloys, e.g., the well known Nb-Mo system⁽³⁾ for which Powell et al. showed that the low T_c alloy Nb_{0.25}Mo_{0.75} ($T_c \approx 0.04$ K) no longer possesses any phonon anomaly. The A-15 superconductors like V₃Si and Nb₃Sn also display a correlation between high values of T_c and the occurrence of a low temperature structural phase transformation⁽⁴⁾ (from the cubic to tetragonal phase), or the existence of anomalous mode softening for the non-transforming compounds. However, even though instability or anomalous phonon softening in many systems appear to be correlated with the occurrence of a high T_c , there also exist some counter examples⁽⁵⁾. Quantitative relations between these experimental facts are more difficult to draw from first principles calculations. However, in the existing model theories, such as the strong coupling theory⁽⁶⁾, the occurrence of soft phonon modes reflected in the variation of the second moment of the phonon frequency, $\langle \omega^2 \rangle$ [defined in ref. 6], does not appear to be sufficient to explain the variation of the electron phonon coupling constant λ which

essentially determines T_c . From the compilation of experimental data, and using his calculated phonon density of states, Weber⁽⁷⁾ showed that a large variation of the electron-phonon matrix elements $\langle i^2 \rangle$ [defined in Ref. 6] is required to explain the variation of λ in the 8 and 9 valence electron TMC. The same conclusions were later reached by Klein and Papaconstantopoulos⁽⁸⁾ using $\langle u^2 \rangle$ given by Weber, and the Gaspari-Gyorffy⁽⁹⁾ expression of the electron-phonon interaction. More recently, after analyzing experimental data, Varma and Dynes⁽¹⁰⁾ also concluded that the transition metals "soft phonon are not responsible for high T_c ".

Since the two physical phenomena, phonon mode softening and high T_c occur concomitantly in the TMC, it is very important to understand the origin of the phonon anomalies in these materials. Several theoretical approaches to the lattice dynamics of the TMC are already available in the literature. Weber, Bilz and Schröder⁽¹¹⁾ and Weber⁽¹²⁾ developed a very successful phenomenological model, reproduced the phonon dispersion curves of the 8 and 9 valence electron TMC and predicted anomalies in some symmetry directions (e.g., the [110] in TaC), which were later confirmed experimentally⁽¹³⁾. Weber⁽¹²⁾ showed that the phonon dispersion curves of the 8 valence electron compounds are well reproduced by a simple shell model with free-electron dielectric screening. However, for the 9 valence electron compounds, the anomalies cannot be reproduced without introducing a new degree of freedom to describe the short range d-d metal ion interaction. In this so-called double shell model (DSM), the anomalies were explained⁽¹²⁾ as being due to a "resonance-like increase of the electronic polarizability" when the metal ions vibrate in phase opposition. The evidence of a certain amount of d metallic charge density of d_{xy} symmetry between the metal ions has been

confirmed by the charge density analysis of Chadí and Cohen⁽¹⁴⁾ resulting from their empirical pseudopotential band structure calculation. Additional evidence that the screening in the 9 valence electron TMC is inadequately described by a free-electron Lindhard function was given by Mostoller⁽¹⁵⁾ who showed, using a pseudopotential to describe the electron-ion interaction and a free electron dielectric screening, that he could reproduce the shapes of the phonon dispersion curves but not the anomalies. Recently, a phenomenological three body force shell model (TSM) was applied successfully to HfC and TaC by Verma and Gupta⁽¹⁶⁾. Whereas the parameters in this model cannot be interpreted in an obvious way as "resonance" effects due to the instability of the metallic d charge density, these authors pointed out that the TSM describes the long range ion-ion interaction which was represented in Weber's DSM by a short range screened ion-electron-ion interaction term. It thus appears that the two models describe the same physical phenomenon.

A different approach for describing the longitudinal acoustic branches of NbC is given by Sinha and Harmon⁽¹⁷⁾ in detail elsewhere in this proceedings. The electron-ion interaction is described in terms of a local pseudopotential and using an ansatz, the dielectric screening matrix is factorized and inverted analytically. The parameters entering into this calculation are determined by a fit to the experimental curves. The transverse branches, which were not obtained because the d orbital overlap was neglected as a simplifying assumption, could in principle be included in the model. We have been informed that a calculation by Hanke⁽¹⁸⁾ et al on NbC, is essentially similar to the work of Sinha and Harmon.

From the previously reported calculations and the physical interpretation of the anomalies as discussed by Weber⁽¹²⁾, the role of the dielectric screening appears to be the essential factor in the occurrence of phonon anomalies; this is also in agreement with the idea of "overscreening" developed by Phillips⁽¹⁹⁾. Due to the complexity of the problem, no ab-initio calculation of the dielectric screening matrix for the TMC has been performed to date.

We have examined the physical information contained in the generalized susceptibility function $\chi(\vec{q})$, which in linear response theory is the response of the conduction electrons to an external perturbation (here, the change in the crystal potential due to the lattice vibrations).⁽²⁰⁾ Let us assume that the lattice is driven into a vibrational mode defined by the wave vector $\vec{q}$. If, for this particular mode, the response function of the conduction electrons of the system shows a divergence, the screening of this vibrational mode will be rather strong and will lead to softening of the mode. This trend can be seen directly from the mathematical expressions. The phonon frequency ω corresponding to a mode $\vec{q}$ is obtained by solving the well-known secular equation:

$$|| D_{KK'}^{\alpha\beta}(\vec{q}) - M_K \omega^2(\vec{q}) \delta_{KK'} \delta_{\alpha\beta} || = 0 \quad , \quad (1)$$

where D is the dynamical matrix for the wave vector $\vec{q}$. The indices α, β refer to the coordinates $1 \leq \alpha \leq 3$; K, K' are the indices of the atoms, M_K their mass. The dynamical matrix can be written as the sum

of two terms, the core-core interaction $\underline{C}$ and the electronic contribution $\underline{E}$

$$\underline{D} = \underline{C} + \underline{E} \quad (2)$$

If, for simplicity we represent the electron-ion interaction by a pseudopotential, the electronic contribution to the dynamical matrix can be written as

$$E_{KK'}^{\alpha\beta}(\vec{q}) = \sum_{\vec{G}, \vec{G}'} \frac{(\vec{q}+\vec{G})_{\alpha}(\vec{q}+\vec{G}')_{\beta}}{V(\vec{q}+\vec{G})} W_K(\vec{q}+\vec{G}) W_{K'}(\vec{q}+\vec{G}') [e^{-1}(\vec{q}+\vec{G}, \vec{q}+\vec{G}') - \delta_{\vec{G}\vec{G}'}] \times e^{i\vec{G} \cdot \vec{r}_K} \cdot e^{-i\vec{G}' \cdot \vec{r}_{K'}} \quad (3)$$

The summation is carried over the reciprocal lattice vectors $\vec{G}$ and $\vec{G}'$, and $W_K(\vec{q}+\vec{G})$ is the Fourier transform of the electron-ion pseudopotential; $\vec{r}_K$ is the position vector of atom K in the unit cell and the dielectric screening matrix $\underline{\epsilon}$ can in turn be expressed in terms of the generalized susceptibility matrix χ :

$$\epsilon(\vec{q}+\vec{G}, \vec{q}+\vec{G}') = \delta_{\vec{G}\vec{G}'} + V(\vec{q}+\vec{G}) \chi(\vec{q}+\vec{G}, \vec{q}+\vec{G}') \quad (4)$$

$V(\vec{q}+\vec{G})$ is the Fourier transform of the electron-electron interaction (including exchange and correlation).

From these expressions and using simplifying assumptions, it can be seen that if χ becomes large, the corresponding phonon frequency is expected to be small, as ω is related to χ through the inverse

of the dielectric screening matrix.

If $E_{\vec{k}}^n$ and $\psi_{\vec{k}}^n$ are respectively the energy and wavefunction of state $\vec{k}$, band index n and $f_{\vec{k}}^n$ is the corresponding Fermi distribution function, the elements of the generalized susceptibility matrix is given by:

$$\chi(\vec{q}+\vec{G}, \vec{q}+\vec{G}') = \sum_{\substack{\vec{k}, \vec{k}' \\ n, n'}} \frac{f_{\vec{k}}^n - f_{\vec{k}'}^{n'}}{E_{\vec{k}'}^{n'} - E_{\vec{k}}^n} \cdot \langle \psi_{\vec{k}}^n | e^{-i(\vec{q}+\vec{G}) \cdot \vec{r}} | \psi_{\vec{k}'}^{n'} \rangle \langle \psi_{\vec{k}}^{n'} | e^{i(\vec{q}+\vec{G}') \cdot \vec{r}} | \psi_{\vec{k}}^n \rangle \quad (5)$$

We have performed an accurate ab-initio determination of the diagonal matrix element $\chi(\vec{q}) = \chi(\vec{q}, \vec{q})$ for several of the 9 and 8 valence electrons TMC: [NbC, TaC, ZrC, HfC] and have found a striking correlation between the existence of large maxima in the band 4 contribution to $\chi(\vec{q})$ for the 9 valence electrons compounds at exactly the $\vec{q}$ values where the phonon anomalies are found experimentally. The generalized susceptibility function of the 8-valence electron compounds is drastically different, does not show any strong maxima, but rather decreases in all symmetry directions from its value at the Γ , the zone center. This result correlates very well with the fact that no anomalies are observed for these compounds and emphasizes the role played by the conduction electron response function in the occurrence of phonon anomalies.

II. Electronic Band Structure, Density of States and Fermi Surfaces

In order to calculate the energy denominator dependence of Eq.(5), we performed a band structure calculation for NbC and TaC (which crystallize in the rocksalt structure) using the Augmented Plane Wave (APW) method. The crystal charge density was obtained by superposition of the neutral atom charge densities obtained from the Herman-Skillman self-consistent atomic program and including 14 shells of neighbors. The original Slater local exchange potential⁽²¹⁾ was used in the determination of the atomic charge densities as well as for the band structure calculation. Expanding the APW wave function in a basis set of 68 plane waves, we obtained a convergence of the order of 1 mRy in the energy eigenvalues. The ab-initio calculation of the valence and conduction band energy eigenvalues was performed at 89 points in the 1/48th irreducible Brillouin zone (BZ). The calculations for both compounds were carried out in an exactly similar fashion and the resulting bands for NbC are plotted in Fig. 1 along some high symmetry directions; similar results were obtained for TaC.⁽²⁰⁾ The two compounds show a great similarity in their band structure as we can expect from the position of the metal atoms in the same column of the periodic table. In Fig. 1, the zero of the energy refers to the constant value of the potential outside the muffin-tin spheres.

The lowest band shown in Fig. 1 is the C-2s band (with some slight admixture of metal states) and is separated from the next group of levels by a direct gap at L.

→ (m, p)

The next three bands above the C-2s band are essentially C-2p states with an important bonding-metal d contribution (and a slight admixture of higher metal states). In both compounds, the C-2p and metal d bands overlap as can be seen in the Γ to X (Δ) direction. This result is in qualitative agreement with the X-ray emission spectra by Ramqvist *et al.*⁽²²⁾ and Källne and Pessa⁽²³⁾. The essential features of the band structure found in this calculation agree with previously reported results by Chadi and Cohen⁽¹⁴⁾, and by Simpson⁽²⁴⁾ using the semi-self-consistent APW method method in the muffin-tin approximation. The main difference between our results and Simpson's is that the latter found a greater overlap between the C-2p and Nb-4d bands. Although a fully self-consistent result would be desirable, it is well known that SCF calculations within the approximation of the muffin-tin potential have to be taken with caution, especially in covalently bonded compounds like NbC as, at each iteration, the charge density is spherically averaged inside the muffin-tin spheres leading to a loss of the directional properties of the bonds at each cycle. Furthermore, the fact that a limited number of points in the BZ were used by Simpson to calculate the charge density at each cycle, can also lead to a substantial loss of accuracy.

A preliminary calculation⁽²⁵⁾ using a molecular cluster model of the form MC_6 was used to understand some features of the bonding mechanism in the solid. The metal "d" states lie essentially above the C-2p band with, of course, some hybridization and overlap as noted above. The "d" band width results from the covalent bonding C-2p-metal "d" states and also a certain

amount of metal d-d interaction, which appears to be an important element in the lattice dynamics of the crystal⁽¹²⁾. The C-2p band width, the d band width and the crystal field splitting at Γ increase slightly from NbC to TaC; this effect can essentially be attributed to a decrease in the lattice constant and can also be predicted in terms of the position of the atomic d level of the metal (which is lower in TaC than in NbC) and consequently interacts more strongly with the C 2p level. The higher s and p states of the metal do not mix strongly with the metal d band. This feature, which is different from what is observed in the corresponding transition metal is characteristic of the formation of an anti-bonding metal s-p states and carbon 2s-2p states in the compound, in agreement with the observation of Mattheiss⁽²⁶⁾ for a similar compound, NbN.

The features of the band structures mentioned above are reflected in the density of states (DOS) shown in Fig. 2 for TaC; a similar DOS was obtained for NbC.⁽²⁰⁾ The energy eigenvalues, calculated ab initio at 89 points in the 1/48th irreducible Brillouin zone (BZ), were fitted by an expansion into a set of 50 symmetrized plane waves. This procedure led to a maximum rms error of $\sim 2\text{mRy}$ for both compounds. The Brillouin zone integration was then carried out using an accurate analytic tetrahedron linear energy method^(27,28) in which the 1/48th irreducible wedge of the BZ was divided into 6144 tetrahedra. The value of the Fermi energy was found to be $E_F = 0.770 \text{ Ry}$ for NbC and $E_F = 0.810 \text{ Ry}$ for TaC. The DOS at E_F is slightly lower for TaC (8.67 states of both spin/Ry-unit cell) than for NbC (9.08 states). The experimental values reported by Toth⁽²⁹⁾ from electronic

specific heat measurements are 9.79 for NbC and 10.88 for TaC. The carbon 2s band is well separated in energy from the C_{2p} -metal d bands, as shown in Fig. 2. At positive energies, the C 2p states, with some admixture of d states characteristic of the covalent metal-ligand bonding, give rise to two peaks. The limited overlap between C 2p and metal d states is responsible for the sharp decrease in the value of the DOS around $E \sim 0.6$ Ry. Then, as we go up in energy, the DOS rises again, due to the increasing contribution of the metal d states belonging essentially to the " t_{2g} " manifold (with, of course, some contribution from C-2p states). The states belonging to the " e_g " manifold overlap those of the t_{2g} manifold but give an important contribution for energies greater than 0.85 Ry for NbC and 0.9 Ry for Ta and contribute to the next main peak in the DOS of height ~ 35 states/Ry-cell. The DOS plotted in Fig. 2 includes only 9-valence and conduction bands. For both compounds, the Fermi energy (E_F) falls in the lower part of the metal 4d (5d) bands essentially in the " t_{2g} " band complex. This is in agreement with the results obtained from different band structure calculations^(14,24) and confirms that these compounds are essentially d type superconductors, in contradiction with a model proposed by Geballe *et al.*⁽³⁰⁾ where the s and p states were assigned the major role at E_F .

It is seen from Fig. 1 that three bands cross the Fermi energy; they belong essentially to the 4d band complex of " t_{2g} " symmetry. If we omit the C 2s band, which is filled and well-separated

in energy, the 3 bands crossing the Fermi energy can be labelled (in increasing values of the energies) as bands 4,5,6. An analysis of the DOS of these bands up to the Fermi energy shows that band 4 plays the dominant role in the Fermi surface (FS) related properties, as it accomodates in both compounds almost the full totality (~96%) of the remaining one "d" electron to be filled.

The cross sections of the FS for the three bands crossing the Fermi energy in NbC are drawn in two high symmetry planes in Fig. 3. Similar cross-sections have been obtained for TaC. The FS of bands 5 and 6 can be described as small electron surfaces centered around Γ ; band 5 Fermi surface has the shape of a deformed "cube" with stretched and rounded corners as can be seen from the cross sections along the Γ to K and the Γ to L directions. Band 6 gives rise to a "cube" with rounded corners of dimension ~ 0.32 in $\frac{2\pi}{a}$ units for both NbC and TaC. Since band 4 is of particular interest for both compounds, we sketch its corresponding Fermi surface in Fig. 4 for NbC in the first BZ; it has a similar shape, with slightly larger volume, for TaC. This FS is a multiply connected "jungle-gym" electron surface which can be roughly characterized, away from Γ , as formed by 6 flattened cylinders with axes ΓX . In fact, as is clearly seen in Fig. 3(a), the dimension of the cross sections of each arm of the "cylinder" perpendicular to the ΓX axes decreases from the point X in the BZ to points closer to Γ . The maximum dimension of the flattened portions of the "cylinders" are spanned by vectors belonging to the star of $\vec{k} = \{0.7, 0.0, 0.0\} \frac{2\pi}{a}$ for NbC, and $\vec{k} = \{0.72, 0.0, 0.0\} \frac{2\pi}{a}$ for TaC, giving rise to "nesting" features of the Fermi surface (nearly parallel pieces

which "nest" into each other upon translation by a well-defined $\vec{k}$ vector). The minimum dimension of the cross sections in the xy plane is $k \sim 0.55 \left(\frac{2\pi}{a}\right)$ for both compounds. The portion of the band 4 Fermi surface sketched in Fig. 4 around Γ in the first Brillouin zone is supplemented by another identical piece, obtained by translation by the reciprocal lattice vector $\vec{G} = (1,1,1)\frac{2\pi}{a}$. The cross section of this piece of Fermi surface appears around the K point of the first BZ, shown in Fig. 3(a), in the ΓXW plane. It can be seen clearly that this cross section displays flat portions and can be characterized as a rounded square. Looking at the cross sections in the ΓXW plane, another vector $\vec{k} \sim \{0.3, 0.0, 0.0\}\frac{2\pi}{a}$ appears also to connect flat portions of the Fermi surface; however, this vector connects portions of different "arms" of the flattened cylinders and consequently, if we look at the spatial configuration, this vector plays a minor role compared to $\vec{k} \sim \{0.7, 0.0, 0.0\}\frac{2\pi}{a}$ in the occurrence of "nesting" features of the band 4 Fermi surface. In the $[110]$ direction, it can be seen from the cross sections of band 4 in the ΓKL plane [see Fig. 3(a)] that an obvious "nesting" vector is $\vec{k} \sim \{0.55, 0.55, 0.0\}\frac{2\pi}{a}$. However, in the $[111]$ direction, a continuous range of vectors $0.7|\Gamma L| < |\vec{k}| < |\Gamma L|$ span a given "arm" of the jungle gym; moreover, two different "arms" having parallel axes can be spanned in the $[111]$ direction by a set of vectors such as $0.6|\Gamma L| < |\vec{k}| < |\Gamma L|$.

The general characteristics of the band 4 Fermi surface obtained in this work for NbC agree with the cross sections available in the literature like the ΓXW plane cross sections shown by Chadi and Cohen⁽¹⁴⁾;

the band 4 FS cross sections of Simpson⁽²⁴⁾ also display similar features to those obtained in the present calculation. This fact shows that the Fermi surface obtained for band 4 is not very sensitive to the atomic configuration used to construct the crystal potential. Recently, similar conclusions were drawn for the Fermi surface of Nb⁽³¹⁾ on the basis of a comparison between a non-self-consistent and self-consistent APW band structure calculation. For TaC, no relativistic corrections were included; however, considering that essentially only the band 4 determines the FS and this band crosses the Fermi energy at steep angles, these effects are expected to be small⁽³²⁾.

III. Generalized Susceptibilities

Using the results of the APW band structure calculations, we calculated the generalized susceptibility function $\chi(\vec{q})$ in the constant matrix elements approximation, defined by,

$$\chi(\vec{q}) = -\sum_{\vec{k}, n, n'} \frac{f_{\vec{k}}^n - f_{\vec{k}+\vec{q}}^{n'}}{E_{\vec{k}}^n - E_{\vec{k}+\vec{q}}^{n'}} \quad (6)$$

where all symbols have been previously defined in Eq.(5). As can be seen from Eq.(6), large contributions to $\chi(\vec{q})$ are expected at those

values of the wave vector $\vec{q}$ connecting states having nearly the same energy and different occupancies, hence maxima in $\chi(\vec{q})$ are expected when large portions of the FS are spanned by a given vector $\vec{q}$ ("nesting" effect) or when parallel bands near E_F are spanned by a $\vec{q}$ vector (so-called "volume" effect).

The necessity of using a very accurate procedure to calculate $\chi(\vec{q})$ was emphasized by Evenson *et al.* ⁽²⁷⁾ To carry out the BZ integration, these authors divided the irreducible wedge of the BZ into microcubes and assumed the energy to be constant inside each microzone; they showed that a coarse mesh could give rise to spurious structures (peaks) when computing the well-known analytic Lindhard function for a free electron gas. In order to avoid such inaccuracies, we adapted to the rocksalt structure, the analytic tetrahedron linear energy method derived by Rath and Freeman ⁽³⁴⁾ as an extension of the tetrahedron scheme devised by Jepsen and Andersen ⁽²⁸⁾ and Lehmann *et al.* ⁽²⁷⁾ for computing density of states. In this method, the irreducible BZ is divided into microzones chosen as tetrahedra. If one assumes, following Gilat-Raubenheimer ⁽³⁵⁾, that the energy can be linearly expanded inside each tetrahedron (in which case the surface of constant energy is a plane), then the contribution to $\chi(\vec{q})$ from each microzone can be obtained from simple analytic expressions involving only the volume of the tetrahedron and the energies at its corners. The accuracy of this method has been discussed at length by Rath and Freeman ⁽³⁴⁾ where model calculations, such as that of the Lindhard function, were found to be in very good agreement with the well-known analytic result. The susceptibility of a "box" energy

surface proposed by Fehlnert and Loly⁽³⁶⁾ was also checked successfully in order to test whether the method can also reproduce the effect of very strong "nesting" features. The average deviation of the entire curve was found to be around 0.75%.

In our calculations for the carbides, we also used the analytic tetrahedron integration method⁽³⁴⁾, with 2048 tetrahedra in the 1/48th BZ. As can be seen from Eq. (6), the intraband contribution ($n=n'$) to the generalized susceptibility function is only non-zero for the 3 bands crossing the Fermi energy. Figs. 5 and 6 display the individual intraband contribution to $\chi(\vec{q})$, from bands 4, 5, and 6 along several symmetry and off-symmetry directions, as well as the total interband contribution in both NbC and TaC. Here $\chi(\vec{q})$ was calculated at 20 equally spaced $\vec{q}$ points for each of the directions plotted in Figs. 5 and 6. In addition, the mesh around each of the maxima was further decreased in order to better define the peaks shown.

The remarkable result of these calculations is the existence of strong structure in the contribution from band 4 to $\chi(\vec{q})$. More specifically, the maxima in $\chi(\vec{q})$, which occur at $\vec{q} = (0.6, 0.0, 0.0)$; $\vec{q} = (0.55, 0.55, 0.0)$, $\vec{q} = (0.5, 0.5, 0.5)$ in $\frac{2\pi}{a}$ units for NbC match exactly with the positions of the dips in the longitudinal acoustic branches of the dispersion curves measured by Smith⁽²⁾ in the [100], [110] and [111] symmetry directions. For TaC, the position of the maxima in the calculated $\chi(\vec{q})$ band 4 contribution, found at $\vec{q}=(0.63, 0.0, 0.0)$, $\vec{q}=(0.55, 0.55, 0.0)$, and $\vec{q}=(0.5, 0.5, 0.5)$, are also in

excellent agreement with experiment for the [110] and [111] directions. Even more remarkable, in the [100] direction, the small shift in the q value at which the anomaly occurs in going from NbC to TaC ($q_{th}=0.60$ vs. 0.63) reproduces the trend in the shift observed experimentally ($q_{exp}=0.60$ vs. 0.65).

We must also emphasize the large magnitude of the calculated maxima in $\chi(\vec{q})$. For band 4, the peaks in [100], [110] and [111] directions show an increase of 33.3%, 55.2%, 91.7% for NbC and an increase of 32%, 53%, 90% for TaC from the value of the function at $q=0$ (which is the contribution from band 4 to the DOS at E_F). A striking feature of these results is that the ratios of these maxima also match closely to the magnitude of the depth of the mode softening - as can be seen by calculating $\omega^2(\text{ZrC}) - \omega^2(\text{NbC})$ or $\omega^2(\text{HfC}) - \omega^2(\text{TaC})$ at those $\vec{q}$ values where anomalies occur for NbC or TaC (note that ZrC and HfC do not possess any phonon anomalies). The calculated peaks are broad, as are the dips observed in the dispersion curves.

A possible correlation between "nesting" vectors and phonon anomalies in the [100] and [110] directions has been proposed previously by Chadi and Cohen.⁽¹⁴⁾ However, as mentioned earlier, both "nesting" (FS) and band structure (or "volume") effects contribute to the position of the maxima singled out in the $\chi(\vec{q})$ calculation. From a visual inspection of the geometrical properties of the FS, some features of the $\chi_4(\vec{q})$ contribution can be interpreted: in the [100] direction, the shoulder in $\chi_4(\vec{q})$ observed around $\vec{q} \approx (0.3, 0.0, 0.0) \frac{2\pi}{a}$ can be associated with the limited "nesting" properties pointed out previously, between different arms of the flattened cylinders; more significant is the sharp decrease of $\chi_4(\vec{q})$ for $\vec{q} > (0.7, 0.0, 0.0) \frac{2\pi}{a}$ which is the maximum dimension of the "arms" of the jungle-gym. The exact location of the peak cannot be predicted by

simple visual inspection of the FS; as mentioned previously, the dimension of the rounded squares cross sections varies between $q = 0.55$ to $q = 0.7$ for NbC and to $q = 0.73$ for TaC. Only an accurate calculation can remove the uncertainty of a qualitative estimate based on FS properties of a predicted structure in $\chi(\vec{q})$. Along the $[110]$ direction, the peak in $\chi_4(\vec{q})$ at $q = (0.55, 0.55, 0.0)$ and the drop in $\chi(\vec{q})$ for larger $\vec{q}$ values, are related to the previously mentioned nesting vector $q = 0.78 \approx 0.55\sqrt{2}$ [see Fig. 3]. The response function of the system contains not only information about FS states ("nesting") but also about band structure effects for states below and above E_F ("volume effects"); it is also obvious that the relative height of the peaks cannot be given at all by FS nesting features even when the "nesting" properties are the dominant factor, as each nesting vector which contributes to a peak must be "weighted" by the portion of surface spanned. For example, in the $[111]$ direction, the sharp increase in $\chi(\vec{q})$ for $0.7|\Gamma L| < q < |\Gamma L|$ can be related to the previously mentioned $\vec{q}$ vectors spanning the Fermi surface in this direction, as well as to band structure contributions, but only the $\chi(\vec{q})$ calculation yields the correct position of the peak.

The intraband contributions to $\chi(\vec{q})$ from bands 5 and 6, plotted separately in Figs. 5 and 6, are small in magnitude and do not show any structure. The corresponding curves can be described as "step" functions, the dimension of the "step" being commensurate with the dimension ($q \sim 0.3$) of the small electron surfaces discussed previously. In all directions, the value of $\chi_n(\vec{q})$ for ($n=5,6$) decreases from its value at the zone center Γ . The total interband contribution to $\chi(\vec{q})$ from

bands 4, 5, and 6, shown at the top of Figs. 5 and 6, is remarkably structureless in the total (as well as in the individual) interband contributions. It is important in the constant matrix elements (ME) approximation to plot and discuss separately the intra- and inter-band contributions, as we will explain below.

As mentioned in the Introduction, Weber interpreted the origin of the soft phonon modes as a "resonance-like increase of the polarizability"; from the $\vec{q}$ dependence of the dynamical matrix, the $\vec{q}$ values at which this resonance occur are expected to span the surface of a cube centered at Γ and of dimension $\sim \frac{2\pi}{a}$. Slight departures from this soft mode surface with a shift towards the zone boundary were expected in Weber's model, from the introduction of nearest neighbors force constants. This model of a "soft" surface has proven to be credible, as predictions of the soft modes in some directions were followed by experimental confirmation; consequently, we thought to be of interest to check whether the predictions made by Weber could be present in a microscopic model in which the polarizability of the conduction electrons is described in terms of the generalized susceptibility function. We studied an arbitrary off-symmetry direction Γ to W defined by $[\xi, \xi/2, 0]$ with $0 \leq \xi \leq 2$. Our results, also presented in Figs. 5 and 6, show that the $\chi_4(\vec{q})$ function has a maximum at $\xi \sim 0.65$ for NbC and TaC in the Γ W direction. Taken together, our calculations show that the maxima of the $\chi_4(\vec{q})$ function lie on the surface of a warped cube in $\vec{q}$ space, centered at Γ and of approximate dimension $1.2(\frac{2\pi}{a})$. This result is in striking agreement with the soft mode surface proposed by Weber starting from an entirely different (an phenomenological) formulation.

The one to one correspondence between the large maxima in the calculated $\chi(\vec{q})$ function and the position of the soft phonon modes leads us to

believe that (for the compounds under study) the essential physical phenomenon which is driving the lattice into soft phonon modes is essentially contained in the electronic response function of the system. Although the possibility of divergences in $\chi(\vec{q})$ leading to phonon anomalies was mentioned by Sinha and Harmon⁽¹⁷⁾ for NbC, they made the simplifying assumption that $\chi(\vec{q})$ was constant and equal to the DOS at E_F . Within the limitation of this approximation and assuming that the ansatz used to factorize ϵ is valid, these authors found that the "bell" shape of the Fourier transform of the assumed electron-ion pseudopotential and the magnitude of the DOS at E_F were the essential elements in reproducing the soft phonon modes. We note that our results are not in contradiction with Sinha and Harmon's work, as their calculation could be reparametrized to take into account the structure of $\chi(\vec{q})$.

As a further test of the role played by structure in the response function in the occurrence of phonon anomalies we calculated $\chi(\vec{q})$ for the 8 valence electrons compounds ZrC and HfC, by applying the rigid band model, respectively, to the NbC and TaC energy band results. The Fermi energy of ZrC and HfC falls in a minimum region of the density of states (DOS), $E_F=0.595$ Ry. and $E_F=0.630$ Ry. respectively for ZrC and HfC. For the 8 valence electrons compounds, four bands cross E_F (bands 1, 2, 3, 4 omitting the C-2s band); the first three bands have essentially a C-2p character. The corresponding intraband and interband contributions to $\chi(\vec{q})$ are plotted in Figs. 7 and 8 along symmetry directions. Unlike the case of NbC and TaC, we find for ZrC and HfC that both the individual and the total intraband contributions to $\chi(\vec{q})$ decrease (in all directions) from the value at $\chi(\vec{q})=0$. This results in a maximum at Γ and, consequently,

in an overscreening at the zone center. These results correlate very well with the experimental results of Smith⁽²⁾ where the optic modes at Γ in ZrC and HfC have a significantly lower value than in NbC and TaC. The decrease at Γ is from ~ 17 THz to ~ 13 THz from NbC to ZrC. The general decrease of $\chi(\vec{q})$ away from Γ is also consistent with the fact that no anomalies are present in this low T_c compound. We thus conclude from this study of the 9- and 8-valence electrons TMC that the phonon anomalies of these compounds can be explained essentially as being due to an anomalous increase in the response function of the conduction electrons, resulting in a strong screening of the corresponding phonon modes.

We are pleased to note that following our first reports^(20,37) of our Fermi surface and $\chi(\vec{q})$ results, Klein et al⁽³⁸⁾ undertook to check out our results using extensions of their unpublished band structure calculations performed in 1974. A $\chi(\vec{q})$ curve for band 4 in the [100] and [111] directions, presented at this meeting by Klein et al⁽³⁸⁾ displays similar features to those obtained by us. Unfortunately, for the [110] direction, Klein et al⁽³⁸⁾ obtained more structure in the band 4 intra-band as well as in the total inter-band contribution. In the absence of their detailed description of their numerical (statistical) integration procedure and its check against well-known analytic expressions such as were used by Rath and Freeman,⁽³⁴⁾ we consider their extra structure to be a further demonstration that a lack of numerical accuracy can lead to spurious peaks, as is well known in the literature concerning $\chi(\vec{q})$ calculations.^(33,39-41)

IV . Role of the Matrix Elements; the Wannier function Representation

In order to assess the variation of the oscillator strength matrix elements which in Eq. (5) multiply the energy dependent term, let us expand the Bloch function ψ_k^n in a set of Wannier function a_n

$$\psi_{\vec{k},n}(\vec{r}) = \frac{1}{\sqrt{N}} \sum_{\vec{l}} e^{i\vec{k} \cdot \vec{R}_{\vec{l}}} \cdot a_n(\vec{r} - \vec{R}_{\vec{l}}), \quad (7)$$

where $\vec{R}_{\vec{l}}$ is the coordinate of site $\vec{l}$ and N the number of unit cells in the crystal. Conversely, the Wannier function can be written as,

$$a_n(\vec{r} - \vec{R}_{\vec{l}}) = \frac{1}{\sqrt{N}} \sum_{\vec{k}} e^{-i\vec{k} \cdot \vec{R}_{\vec{l}}} \cdot \psi_{\vec{k},n}(\vec{r}). \quad (8)$$

Using the expansion of Eq. (7) in Eq. (5) and performing the lattice summation, Eq. (5) becomes rigorously:

$$\chi(\vec{q}+\vec{G}, \vec{q}+\vec{G}') = \sum_{\substack{\vec{k}, \vec{k}' \\ n, n'}} \frac{f_{\vec{k}}^n - f_{\vec{k}'}^{n'}}{E_{\vec{k}}^{n'} - E_{\vec{k}}^n} \sum_{\vec{l}, \vec{l}'} e^{i\vec{k} \cdot \vec{R}_{\vec{l}}} \cdot e^{i\vec{k}' \cdot \vec{R}_{\vec{l}'}}.$$

$$\langle a_n(\vec{r} - \vec{R}_{\vec{l}}) | e^{-i(\vec{q}+\vec{G}) \cdot \vec{r}} | a_{n'}(\vec{r}) \rangle = \langle a_{n'}(\vec{r}) | e^{i(\vec{q}+\vec{G}') \cdot \vec{r}} | a_n(\vec{r} - \vec{R}_{\vec{l}}) \rangle, \quad (9)$$

with the condition $\vec{k}' = \vec{k} + \vec{q} + \vec{H}$ (10) $\vec{H}$ being a reciprocal lattice vector which brings $\vec{k} + \vec{q}$ to the 1st BZ. If we now make the approximation of neglecting the overlap between sites $\vec{l}$ and $\vec{l}'$ Eq. (9) can be written in a simpler form:

$$\chi(\vec{q}+\vec{G}, \vec{q}+\vec{G}') = \sum_{\vec{k}, n, n'} \frac{f_{\vec{k}}^n - f_{\vec{k}+\vec{q}}^{n'}}{E_{\vec{k}+\vec{q}}^{n'} - E_{\vec{k}}^n} \langle a_n(\vec{r}) | e^{-i(\vec{q}+\vec{G}) \cdot \vec{r}} | a_{n'}(\vec{r}) \rangle.$$

$$\langle a_{n'}(\vec{r}) | e^{i(\vec{q}+\vec{G}') \cdot \vec{r}} | a_n(\vec{r}) \rangle. \quad (11)$$

In Eq. (11) unlike in Eq. (5), the matrix elements no longer depend upon $\vec{k}$ and $\vec{k}'$, and it is easier to make predictions about their variation, particularly in the $\vec{G}=\vec{G}'=0$ limit (normal processes). We can see that for the element $\chi(\vec{q},\vec{q})$, the energy dependent term will be multiplied by the square of a form factor, which is a slowly varying function of $\vec{q}$. Keeping in mind the orthogonality relations satisfied by the Wannier functions, one can see from Eq. (11) that only the intraband ($n=n'$) part contributes to $\chi(\vec{q},\vec{q})$ in the $\vec{q} \rightarrow 0$ limit. Generally speaking, the dominant contribution to $\chi(\vec{q},\vec{q})$ will be derived from the intraband part and the effect of the matrix elements will be to very much suppress the interband part since for these elements $\vec{q}$ is rather small (restricted to the first BZ). The interband part can be expected to play an important role only if there is a very strong peak at some wave vector⁽³⁹⁾, but this is not the case here. Since normal processes (i.e., terms containing $\vec{G}=\vec{G}'=0$) play a major role in determining the longitudinal branches, we believe that the anomalies observed in the longitudinal acoustic branches can be explained in terms of the behavior of the diagonal elements $\chi(\vec{q},\vec{q})$ of the susceptibility matrix $\chi(\vec{q}+\vec{G}, \vec{q}+\vec{G}')$. Some contribution will, of course, come also from the Umklapp processes as well as from local field corrections ($\vec{G},\vec{G}' \neq 0$).

The possibly important role played by the matrix elements (ME) for several transition metals has been stressed by several authors:⁽³⁹⁻⁴¹⁾ Gupta and Sinha⁽³⁹⁾ (for Cr), and Gupta and Freeman⁽⁴¹⁾ (for Sc) make an explicit use of the APW Bloch functions while Cooke et al.⁽⁴⁰⁾ (for Nb) calculate the matrix elements in the tight binding approximation. In the case of NbC and TaC, we can see from Figs. 5 and 6 that the interband value (without ME) provides a large background for all $\vec{q}$ values,

ranging from ~ 16 to 20 states/Ry unit cell; this is about 2 times larger than the DOS at E_F . It is well known that the large value of the interband contribution at $\vec{q}=0$ is zero when ME are included. Moreover, from all previously reported results with non-constant ME, ⁽³⁹⁻⁴¹⁾ it is seen that the background is largely suppressed for all $\vec{q}$ values. [For example, whereas $\chi(\vec{q})$ without ME in Cr ranges from 132 to 140 states/Ry. atom, it never exceeds 9 states/Ry. atom when the ME are included (due to a drastic reduction of the interband value) and so the variation of $\chi(\vec{q})$ (about 8 states/Ry. atom) remains unaffected by the inclusion of ME. Similarly, $\chi(\vec{q})$ without ME for Nb varies between ~ 60 to ~ 68 states/atom-Ry-spin in the ΓH direction while the result with ME varies between ~ 11 (at $q=0$) to 3.8 states/atom-Ry-spin at H.]

For this reason, and because the interband contribution without ME is remarkably structureless, we do not expect the interband part with ME to give rise to sharp structure. On the other hand, the inclusion of ME into the intraband contribution would modify the results shown in Figs. 5 and 6 by only a slowly varying function (essentially the square of the form factor), as discussed previously. But if we recall the large heights of the peaks emphasized earlier, it seems very improbable that the ME could smear out the strong structure observed without ME, and so we do not expect our general conclusions to be severely affected.

V. Conclusion

Using detailed ab-initio APW band structure calculations, the FS of the 9-valence electron TMC: NbC and TaC, were fully investigated and revealed remarkable nesting properties,⁽¹⁴⁾ which contribute, together with band structure effects, to a strongly $\vec{q}$ dependent generalized susceptibility function of the conduction electrons. The large peaks in the response function correlate exactly with the position of the phonon anomalies observed experimentally and the locus of the maxima [a warped cube of dimension $\sim 1.2(\frac{2\pi}{a})$] in $\chi(\vec{q})$ is in striking agreement with the soft mode surface proposed by Weber.⁽¹²⁾ It appears from these results that the phonon anomalies in the TMC can be essentially interpreted as due to an "overscreening effect"⁽¹⁹⁾ originating from a resonancelike increase of the response function of the system. The important role of the diagonal elements $\chi(\vec{q}, \vec{q})$ of the susceptibility matrix (which are the only elements calculated here) in the onset of phonon softening was further checked successfully for the 8-valence electron compounds which do not show peaks in $\chi(\vec{q})$ and do not possess any anomalies.

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Figure Captions

- Fig. 1. The energy bands of NbC ($a=8.4472$ au) along several symmetry directions. The zero of energy corresponds to the averaged potential in the interstitial region.
- Fig. 2. The density of states of TaC for 9 bands (including the C-2s band).
- Fig. 3. Fermi surface cross sections of NbC.
a) band 4; b) band 5; c) band 6
The bands are labeled omitting the C-2s band. The hatched portions show the occupied regions.
- Fig. 4. The band 4 Fermi surface of NbC in the first Brillouin zone.
- Fig. 5. The generalized susceptibility $\chi(\vec{q})$ of NbC along several symmetry and off-symmetry directions a) the intraband contribution from band 6; b) the intraband contribution from band 5; c) the intraband contribution from band 4 and d) the total interband contribution from bands 4, 5, 6.
- Fig. 6. The generalized susceptibility $\chi(\vec{q})$ of TaC along several symmetry and off-symmetry directions: a) the intraband contribution from band 6; b) the intraband contribution from band 5; c) the intraband contribution from band 4; and d) the total interband contribution from bands 4, 5, 6.
- Fig. 7. The generalized susceptibility $\chi(\vec{q})$ of ZrC along some symmetry directions: the total intraband contribution from all 4 bands crossing E_F (lower curve) and the corresponding total interband contribution (upper curve).
- Fig. 8. The generalized susceptibility $\chi(\vec{q})$ of HfC along some symmetry directions: the total intraband contribution from all 4 bands crossing E_F (lower curve) and the corresponding total interband contribution (upper curve).

Nb C

Fig. 2

Fig. 3(a)

Fig. 3(b)

Fig. 3(c)

Fig. 4

Fig. 5

Fig. 6

Fig. 7

Fig. 8