Superconductivity and phonon softening. III. Relation between electron bands and phonons in Nb, Mo, and their alloys*

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Calculations are presented by $\chi_1(\vec{Q})$ and $\chi_2(\vec{Q},\omega)$ for Nb, Mo, and alloys in the rigid-band model. The matrix elements are set to 1. The results for Nb agree with a previous calculation by Cooke, Davis, and Mostoller. An empirical linear relation is found between $\chi_1(\vec{Q})$ and $d\chi_2(\vec{Q},0)/d\omega$. This relation leads to a simple formula relating the superconducting coupling constant (λ) to the phonon frequencies. However, we are unable to evaluate the terms in this formula with sufficient accuracy to calculate λ.

I. INTRODUCTION

It is not yet clear whether the present microscopic formulation of lattice dynamics[1] is simple or accurate enough to allow realistic calculations for *d*-band metals with phonon anomalies such as niobium. Empirically,[2,3] the anomalies are correlated with high superconducting transition temperatures T_c. This leads one to believe that the mechanism for phonon anomalies may also be a mechanism for high T_c's. A stronger formulation is that soft phonons cause the high T_c.[4] The denial of this statement is also sometimes made.[5] We avoid this "chicken-egg" controversy by using the weaker formulation of the soft-phonon–high-T_c connection.

The formula for the phonon self-energy $\underline{\Pi}$ (which is also the electronic contribution to the dynamical matrix) can be written[1]

$$\underline{\Pi}(\vec{Q},\omega) = -2\sum_{\vec{k}nn'} \frac{f_{\vec{k}n} - f_{\vec{k}+\vec{Q}n'}}{\epsilon_{\vec{k}+\vec{Q}n'} - \epsilon_{\vec{k}n} - \hbar\omega - i\delta}\, \underline{\overline{M}}^2_{\vec{k}n,\vec{k}+\vec{Q}n'}, \tag{1}$$

where $f_{\vec{k}n}$ is the Fermi occupation factor for an electron of wave vector and band index $(\vec{k}n)$ and energy $\epsilon_{\vec{k}n}$. The effective matrix element $\underline{\overline{M}}$ is defined by

$$\underline{\overline{M}}^2_{kn,k'n'} \equiv \langle \vec{k}'n' | \delta V^b/\delta\vec{r} | \vec{k}n\rangle \langle \vec{k}n | \delta V^{sc}/\delta\vec{r} | \vec{k}n'\rangle , \tag{2}$$

where $\delta V^b/\delta\vec{r}$ is the change in the bare electron-ion potential per unit displacement of a single atom, and $\delta V^{sc}/\delta\vec{r}$ is the same except corrected for the screening, exchange, and correlation effects felt by a conduction electron. The self-energy is related to the phonon frequency ω_Q and width γ_Q by

$$\omega_Q^2 = \overline{\Omega}_Q^2 + 2\overline{\Omega}_Q \Pi_1(\vec{Q},\omega_Q), \tag{3}$$

$$\omega_Q \gamma_Q = -\overline{\Omega}_Q \Pi_2(\vec{Q},\omega_Q), \tag{4}$$

where Q is shorthand for wave number and branch index $(\vec{Q}\nu)$. Here and below the subscript 1 (2) denotes the real (imaginary) part and the matrix nature of Π has been disregarded for simplicity. The frequency spectrum $\overline{\Omega}_Q$ is that which would result if the electrons did not respond to ion displacements.

It was pointed out by one of us[6] that a simple linear relation exists between the width γ_Q or Π_2 and the coupling constant λ for superconductivity. Unfortunately, γ_Q is not directly measureable with present technology except in certain especially favorable cases.[7] Two previous papers[8] (denoted I and II) have attempted to establish an approximate linear relation between Π_1 (and thus ω^2) and Π_2 (and thus λ). A difficulty immediately occurs, namely, Π_2 is determined by electronic states only very near the Fermi level, whereas Π_1 contains virtual transitions to states both near and far from the Fermi level. The high-energy transitions must be subtracted out if a useful linear relation is to be obtained. Determining the manner and extent to which this can be carried out in high-temperature superconductors is the purpose of this series of papers. In I, a model for the subtraction was proposed (with little microscopic justification) which leads to a formula relating the difference $\Delta\lambda \equiv \lambda_A - \lambda_B$ between two similar superconductors, denoted *A* and *B*, to the differences in their observed phonon spectra. Evaluation[9] of the expression derived in I for transition metals indicated the correct trends but since little was known concerning the validity of the assumptions for these metals, the agreement was viewed as tentative. In II it was shown that a similar model (with more microscopic justification) worked well for lead alloys. In this paper detailed microscopic calculations are presented which indicate that a model similar to that used in I is justified in the bcc transition-metal alloy system $Nb_{1-x}Mo_x$.

We are unable to evaluate $\underline{\Pi}$ properly from Eq. (1) because the matrix element $\underline{\overline{M}}$ is formidably difficult to evaluate. We calculate instead a function $\chi(\vec{Q}\omega)$

equal to $\underline{\Pi}$ if the matrix elements $\overline{M}^2$ are set equal to $(-\frac{1}{2})\underline{1}$,

$$\chi(\vec{Q},\omega) \equiv \sum_{knn'} \frac{f_{\vec{k}n} - f_{\vec{k}+\vec{Q},n'}}{\epsilon_{\vec{k}+\vec{Q},n'} - \epsilon_{\vec{k}n} - \hbar\omega - i\delta}. \tag{5}$$

A recent calculation of $\chi_1(\vec{Q},0)$ for Nb by Cooke, Davis, and Mostoller[10] (CDM) shows very little correlation with ω_Q^2 and thus demonstrates that $\overline{M}$ is not a smooth function of $\vec{Q}$. In Sec. II we report calculations of $\chi_1(\vec{Q},0)$ and $\chi_2(\vec{Q},\omega)$ for both Nb and Mo as well as some intermediate cases (rigid-band alloys) which confirm the CDM results and which also exhibit previously unreported regularities that we believe will persist in a more realistic theory. These regularities support and illuminate the conjectures of Papers I and II.

II. CALCULATIONS OF χ

The calculation of χ from Eq. (5) is time and space consuming even on large modern computers. We have chosen a Slater-Koster parametrization scheme (described elsewhere[11]) in order to generate accurate eigenvalues ϵ_{kn} rapidly. A 31-parameter model using nine bands (s, p, and d) gives an excellent fit (7-mRy-rms deviation for the lowest six bands in the zone) to the augemented-plane-wave (APW) calculations for Mattheiss[12] for Nb and Petroff and Viswanathan[13] for Mo. A calculation of $\chi_2(0,\omega)$ using these fitted bands has been reported[14] and gives an excellent qualitative description of the measured optical properties of Nb and Mo. A rigid-band model based on the Nb bands agrees with the Mo bands to about 3%. In this paper we use a rigid-band model for both elements and their alloys. The use of the rigid-band model for the alloys is supported by specific-heat data,[11] and has been justified by recent theoretical calculations[15] using the coherent-potential approximation, but is only partially supported by optical measurements.[16]

Our calculations of $\chi_1(\vec{Q},0)$ for $\vec{Q}$ along the [100] direction are shown in Fig. 1. This calculation and others described below are the result[11,17] of Gilat–Raubenheimer-like integrations over the Brillouin zone. There is good agreement with a very similar but independent calculation for Nb by CDM,[10] especially after introducing a small constant shift of 8.0 units which presumably compensates for a small difference in the maximum energy used in calculating χ_1. We agree with the conclusion of CDM that little correspondence can be seen between the structure of $\chi_1(\vec{Q})$ and the measured features in ω_Q^2 for Nb. For Mo, the strongest feature in ω_Q^2 in the [100] direction is a very sharp Kohn anomaly near the zone boundary; a similar feature occurs in W and Cr and is believed to be the source of the incommensurate antiferromagnetism of Cr. Our calculation of χ_1 for Mo

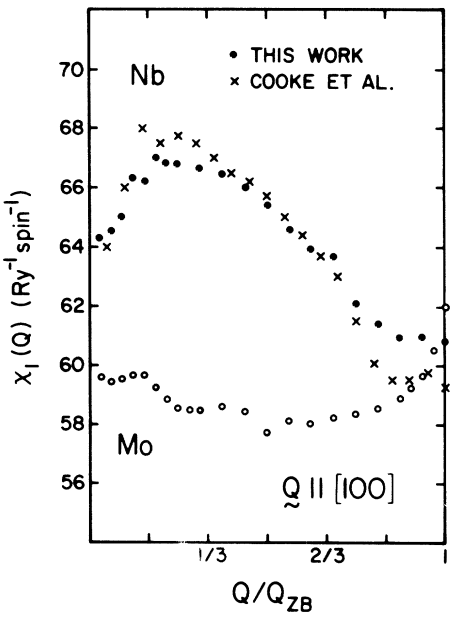

FIG. 1. $\chi_1(\vec{Q},0)$ as a function of $\vec{Q}$ in the [100] direction out to the zone boundary $|\vec{Q}_{ZB}| = 2\pi/a$. The closed and open circles are the present calculation for Nb and Mo, respectively, with a small constant (8.0) added to bring agreement with the work of Cooke *et al.* (Ref. 10) shown as crosses for Nb. The added constant presumably comes from a higher energy cutoff used in the calculation of χ in Ref. 10.

shows a sharp increase of about 5% just at the location of the Kohn anomaly. We have verified[11] that this increase arises from transitions near the Fermi level and is sensitive to small changes in Fermi energy, as expected for a Kohn anomaly. CDM have found for Nb that including matrix elements of $\exp(i\vec{Q}\cdot\vec{r})$ in the calculation of χ_1 does not remove the discrepancies with ω_Q^2 of niobium. The matrix element $\overline{M}$ which should be included is much more complicated than $\exp(i\vec{Q}\cdot\vec{r})$, so the lack of improvement is not too surprising.

Although the correspondence between the real quantities ω_Q^2 and χ_1 is disappointing, it is possible that a better correspondence occurs between the imaginary parts $\omega_Q\gamma_Q$ and $\chi_2(\vec{Q},\omega_Q) \approx \omega_Q(d/d\omega)\chi_2(\vec{Q},0)$. The behavior of γ_Q has not been directly measured, but we expect some correspondence between the $\vec{Q}$ dependence of γ_Q and of ω_Q^2. To test this, we have calculated a function

$$I_{\vec{Q}}(E,E') \equiv \sum_{knn'} \delta(\epsilon_{\vec{k}n} - E)\,\delta(\epsilon_{\vec{k}+\vec{Q}n} - E'). \tag{6}$$

The imaginary part $\chi_2(\vec{Q},\omega)$ at low frequencies is related to $I_{\vec{Q}}$ evaluated at the Fermi energy ϵ_F,

$$\frac{1}{\pi}\frac{d}{d\omega}\chi_2(\vec{Q},\omega)\bigg|_{\omega=0} = I_{\vec{Q}}(\epsilon_F,\epsilon_I) \equiv I_{\vec{Q}}. \tag{7}$$

The behavior of $I_{\vec{Q}}$ as a function of $\vec{Q}$ and ϵ_F is shown in Fig. 2. The meaning of I_Q is that it measures the number of electron-hole states available with wave vector $\vec{Q}$ at the Fermi level. As ϵ_F varies, $I_{\vec{Q}}$ scales roughly as the square of electron density of states $N(\epsilon_F)^2$ and the Brillouin zone average of $I_{\vec{Q}}$ is exactly $N(\epsilon_F)^2$. This explains the minimum in $I_{\vec{Q}}$ when E_F lies between the Fermi energy of Nb and Mo, because there is a minimum in $N(\epsilon_F)$ there. The structure in $I_{\vec{Q}}$ as $\vec{Q}$ is varied unfortunately also does not correlate with $\omega_{\vec{Q}}^2$ (except for the zone-boundary Kohn anomaly in Mo).

The central result of this paper is a surprisingly strong correspondence which appears when one compares the behavior as a function of $\vec{Q}$ of $\chi_1(\vec{Q},0)$ in Fig. 1 and $I_{\vec{Q}}(\epsilon_F,\epsilon_F)$ in Fig. 2. To illustrate this better, a scatter plot is shown in Fig. 3 of χ_1 and $I_{\vec{Q}}$ for all available values of $\vec{Q}$. Empirically, we find

$$\chi_1(\vec{Q},0)-\bar{\chi}\cong 2\bar{\omega} I_{\vec{Q}}(\epsilon_F,\epsilon_F), \tag{8}$$

with the empirical values $\bar{\chi}=56$ Ry^{-1}spin^{-1} and $2\bar{\omega}=0.044$ Ry independent of $\vec{Q}$. The accuracy of this empirical relation is more easily seen in Fig. 4 where both the left- and right-hand sides of relation (8) are plotted as a function of $|\vec{Q}|$. The accuracy of this relation is quite surprising considering that $\chi_1(\vec{Q},0)$ is a sum over electronic states of all energies while $I_{\vec{Q}}(\epsilon_F,\epsilon_F)$ comes strictly from electrons at the Fermi surface. However, we can qualitatively understand the behavior (8) in the following way. At low frequencies, $\chi_2(\vec{Q},\omega)$ is linear in ω with a slope $\pi I_{\vec{Q}}(\epsilon_F,\epsilon_F)$. Suppose this behavior persists up to the frequency $\bar{\omega}$, and above that frequency $\chi_2(\vec{Q},\omega)$ is independent of Q and equal to say $\bar{\chi}_2(\omega)$. Then from the Kramers-

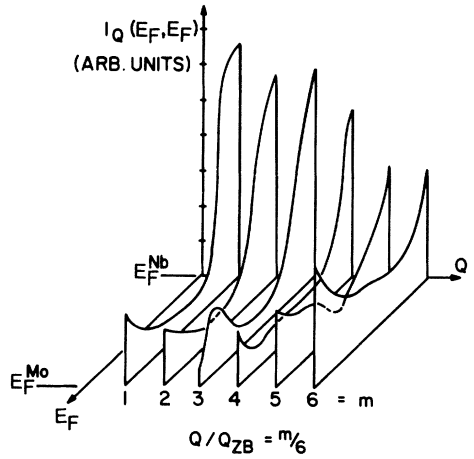

FIG. 2. Electron-hole pair density $I_{\vec{Q}}(E_F,E_F)$ as a function of $\vec{Q}$ along the [100] direction and as a function of Fermi level between Nb and Mo. The minimum between Nb and Mo corresponds to the density-of-states minimum.

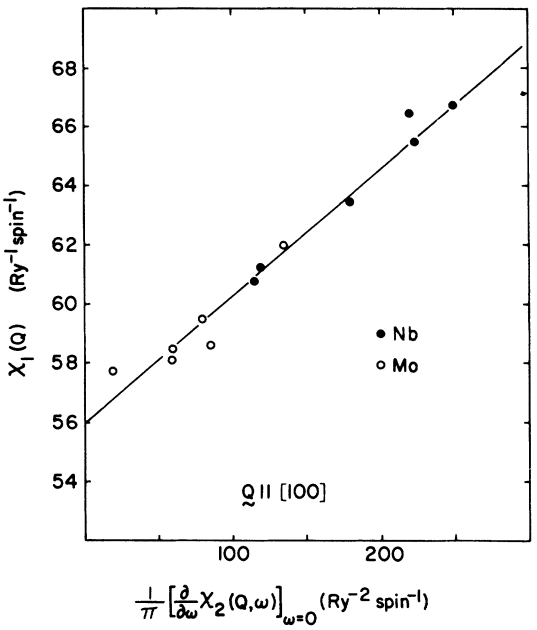

FIG. 3. Scatter plot of $\chi_1(\vec{Q},0)$ plotted vs

$$I_{\vec{Q}}(\epsilon_F,\epsilon_F)=(1/\pi)[(d/d\omega)\chi_2(\vec{Q},\omega)]_{\omega=0}.$$

All available values of $\vec{Q}$ for both Nb and Mo are represented as closed and open circles, respectively.

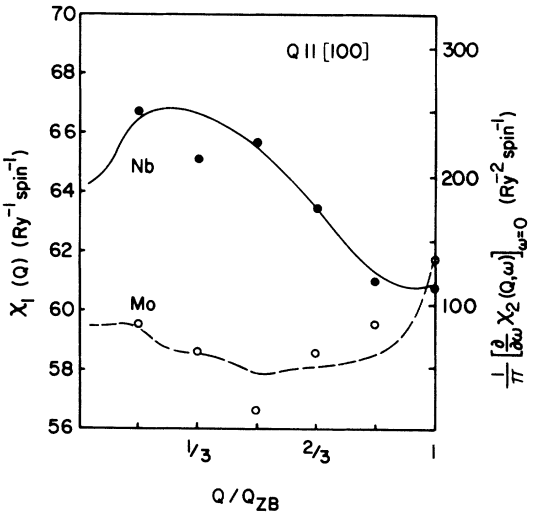

FIG. 4. Left-hand side of relation (8) is plotted (using the left-hand scale) as a function of wave vector with solid and dashed lines, respectively, for Nb and Mo. The right-hand side of relation (8) is plotted (on the right-hand scale) using closed and open circles for Nb and Mo.

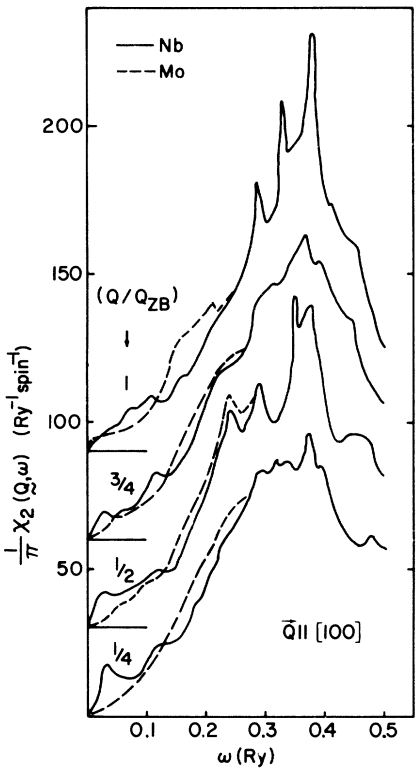

FIG. 5. Imaginary part $(1/\pi)\chi_2(\vec{Q},\omega)$ of the single-spin susceptibility plotted vs the energy $\omega(\hbar=1)$ for four values of the wave vector $\vec{Q}$ in the [100] direction, for Nb (solid lines) and Mo (broken lines). Note that all curves are linear for $\omega \leq 0.025$ Ry and that the curves for Nb and Mo are identical for $\omega > 0.25$Ry.

Kronig relation we find exactly the result (8) for χ_1, with the constant $\bar{\chi}$ given by

$$\bar{\chi} = \frac{2}{\pi}\int_{\omega}^{\infty} d\omega' \frac{\chi_2(\omega')}{\omega'}. \tag{9}$$

Our calculated values of $\chi_2(\vec{Q},\omega)$ are shown in Fig. 5 for four different values of $\vec{Q}$. In Nb it is particularly evident that $\bar{\omega} \sim 0.02$–0.03 Ry does roughly divide a low-frequency linear regime with large variation with $\vec{Q}$ from a complicated large ω regime with smaller variation as a function of $\vec{Q}$. In Mo there is less evidence for such a model, and also weaker evidence for the accuracy of Eq. (8). It is noteworthy that above $\omega \sim 0.25$ Ry, χ_2 for Nb and Mo are almost undistinguishable. The energy 0.25 Ry corresponds to twice the difference in Fermi energy $2\Delta\epsilon_f$. Over the range $0 < \omega < \Delta\epsilon_f$, Nb has a larger χ_2 because of the larger density of states near ϵ_f. However, for $\Delta\epsilon_f < \omega < 2\Delta\epsilon_f$, Mo has a large χ_2, partly because the states near ϵ_f^{Nb} become accessible.

Qualitative reasons for the $\vec{Q}$ independence of χ_2 at large ω and the value 0.022 Ry for the cutoff can be constructed as follows. The electronic density of states of Nb and Mo shows five overlapping peaks (at roughly 0.5, 0.6, 0.7, 0.9, and 1.0 Ry using the zero of Ref. 12). These peaks contain roughly one electron per spin,atom each. This is most easily seen by making a band-by-band decomposition of $N(\epsilon)$, as in Ref. 11. The average peak width is $\gtrsim 0.1$ Ry. The contribution to $\chi_1(\vec{Q},0)$ from higher ω transitions contains energy denominators $\epsilon_{\vec{k}+\vec{Q}_i} - \epsilon_{\vec{k}j}$ which do not vary much with $\vec{Q}$ since the energies are localized in the peaks i and j. Only when peaks i and j begin to overlap (and especially if they are the same) does the $\vec{Q}$ dependence have a relatively large importance. Thus most of the $\vec{Q}$ dependence should come from small ω transitions, within say a half-width ($\lesssim 0.05$ Ry) of a peak. As was noted[14] to be the case for optical ($\vec{Q}=0$) transitions, the structure in $\chi_2(\vec{Q},\omega)$ is dominated by transitions with both initial and final states near a van Hove singularity in $N(\epsilon)$. This can account for the effects of intraband ($i=j$) transitions peaking at the somewhat lower value of $\bar{\omega}=0.022$ Ry.

III. INSIGHTS TOWARD A MORE COMPLETE THEORY

The calculations of Sec. II establish an empirical relation (8) obeyed by the susceptibility χ; we can expect that a similar relation will hold for the true self-energy Π, namely,

$$\Pi_1(\vec{Q},0) = \Pi_L(\vec{Q}) + \bar{\Pi}_1(\vec{Q}). \tag{10}$$

Here Π_L arises from transitions $\sim \pm\hbar\bar{\omega}$ of the Fermi level and $\bar{\Pi}_1$ represents the contributions from higher energy. Unlike Eq. (8) for χ, where $\bar{\chi}$ was independent of $\vec{Q}$, in Eq. (10) we have no arguments to justify neglecting the $\vec{Q}$ dependence of $\bar{\Pi}_1$. The previous arguments tell us that there is a cutoff energy $\hbar\bar{\omega}$ such that for $\omega > \bar{\omega}$, the $\vec{Q}$ dependence of Π_2 comes only from matrix elements, and is independent of the specific shape of the electron dispersion. Since Π_2 is linear for small ω, it follows from the Kramers-Kronig relation that, for $\vec{Q}$ not too small,

$$\Pi_1(\vec{Q}) = -(2/\pi)(\bar{\omega}/\bar{\Omega}_Q)\gamma_Q. \tag{11}$$

where $\gamma_Q/\bar{\Omega}_Q$ is the slope of $-\Pi_2(\vec{Q},\omega)$ at $\omega=0$. The fact that $\bar{\omega}$ is independent of $\vec{Q}$ is an empirical observation which must in fact break down if $\vec{Q}$ is very small. The maximum intraband energy goes to zero as $|\vec{Q}|v_f$ as $|\vec{Q}|$ goes to zero; this defines a $|\vec{Q}|$ cut off $\bar{Q} \equiv \bar{\omega}/v_f$ below which $\bar{\omega}$ must become linear in $\vec{Q}$. For Nb we estimate[11] $v_f = 0.62\times10^8$cm/sec, which gives $\bar{Q} = 0.7\times10^7$ cm^{-1} (using $\bar{\omega}=0.022$Ry). This corresponds to 4% of $2\pi/a$, or only a part in 10^4 of the Brillouin-zone volume.

Combining Eqs. (10) and (11) gives a result identi-

cal to the model of Paper I except that we fix ω by actual calculations of χ rather than by guessing. Using also Eqs. (3) and (4) gives a desired linear relationships between the phonon softening and the phonon width

$$\Omega_Q^2 - \omega_Q^2 = (4\bar{\omega}/\pi)\gamma_Q. \tag{12}$$

The softening is relative to the reference spectrum Ω_Q given by

$$\Omega_Q^2 = \bar{\Omega}_Q^2 + 2\bar{\Omega}_Q \bar{\Pi}_1(Q). \tag{13}$$

The exact relation between the electron-phonon coupling constant λ and γ_0 is[6]

$$\lambda = \frac{2}{\pi N(\epsilon_F)} \sum_{\vec{Q}\nu} \frac{\gamma_{\vec{Q}\nu}}{\hbar\omega_{q\nu}^2}, \tag{14}$$

where ν runs over the three phonon branches. Inserting (12) into (14) we obtain a formula for λ,

$$\lambda = [2\hbar\bar{\omega}N(\epsilon_F)]^{-1} \sum_{\vec{Q}\nu} \left(\frac{\Omega_{Q\nu}^2}{\omega_{Q\nu}^2} - 1 \right). \tag{15}$$

The error from taking $\bar{\omega}$ independent of $\vec{Q}$ for small $\vec{Q}$ is negligible in this formula.

Equation (15) establishes a semiempirical expression for λ. All quantities in (14) are accessible to experiment except $\bar{\omega}$ (which is fixed at 0.022 Ry by our calculation) and the reference spectrum $\Omega_{\vec{Q}\nu}$. Rigorously $\Omega_{\vec{Q}\nu}$ is the phonon spectrum that would result if virtual transitions with energy denominators less than $\hbar\bar{\omega}$ were omitted from (1). Unfortunately $\Omega_{\vec{Q}\nu}$ is nearly as difficult to calculate as is the experimental spectrum $\omega_{\vec{Q}\nu}$, and further progress depends on a sufficiently accurate guess of the reference spectrum. In Paper I it was posited that, inasmuch as any extra ionic charge in the bare spectrum $\bar{\Omega}_Q$ in Eq. (13) will give a balancing contribution to the renormalization $\bar{\Pi}$, the reference spectrum Ω_Q can be taken as constant within a given system. We modify this position only by noting that any volume change in the system must be carefully taken into account. The importance of the volume correction warrants a short digression.

The reference spectrum (13) is determined by the bare spectrum $\bar{\Omega}_Q$ and the self-energy $\bar{\Pi}$. The bare spectrum is largely dependent on the ionic plasma frequency, whose square depends inversely on the volume V. The self-energy depends on the volume both through a (bandwidth)$^{-1}$ factor arising from the energy denominator and, in a more obscure but no less important way, through the potential gradient entering the electron-phonon matrix element. As the reference spectrum will not differ greatly from the observed frequencies $\omega_{\vec{Q}\nu}$, it is reasonable to expect its volume dependence to be similar. Thus the quantity $\Omega_{\vec{Q}\nu}^2$ entering the semiempirical relation (15) will depend on the Grüneisen exponent γ in accordance with $V^{-2\gamma}$. The measured value[18] $\gamma = -1.57$ for the Nb-Mo system leads to a difference in reference spectra of

$$(V^{\mathrm{Mo}}/V^{\mathrm{Nb}})^{-2\gamma} \simeq 0.6. \tag{16}$$

and it becomes apparent how crucial the volume correction will be in evaluating the expression (15).

Our experience has been that with presently available information, $\Omega_Q^2 - \omega_Q^2$ is too uncertain to make (15) a useful relation. Sufficient uncertainty occurs in both Ω_Q^2 and ω_Q^2 that the resulting values of λ from Eq. (8) have only semiqualitative significance. The phonon spectra along symmetry directions have been measured for $\mathrm{Nb}_{1-x}\mathrm{Mo}_x$ ($x = 0.0, 0.15, 0.35, 0.41, 0.56, 0.75, 0.91, 1.0$) by Powell, Martel, and Woods.[19] We have found that the inevitable extrapolations off symmetry directions give the Brillouin-zone averages appearing in (15) a surprisingly large dependence on the model used in representing the spectra. Neither have we succeeded in constructing a reference spectrum which is believable to the necessary accuracy, although certain clues are available from the alloy data. In the $\mathrm{Nb}_x\mathrm{Mo}_{1-x}$ system the average of $(\Omega_{\vec{Q}\nu}^2/\omega_{\vec{Q}\nu}^2 - 1)$, equal to $\frac{2}{3}\hbar\bar{\omega}N(\epsilon_F)\lambda \equiv \Lambda$, reaches a minimum near $x \simeq 0.6$, where $\Lambda = 0.01$. Thus for this alloy the reference spectrum is virtually identical to the experimental spectrum which is smooth and typical of a bcc simple metal.[20] The simplest approach is to assume that this shape for the reference spectrum will persist through the alloy system. However, this ansatz, together with a volume-dependent magnitude, does not appear to give an accurate enough reference spectrum to be of use in (15).

Our conclusions are as follows: (i) we find an empirical linear relation between χ_1 and $d\chi_2/d\omega$ which strongly suggests that a linear relation exists between γ_Q and ω_Q^2; (ii) a model similar to those of Papers I and II appears justified for Nb and Mo, but the resulting formula is too sensitive to small variations in the various unknowns.

Although the conclusions are pessimistic about prospects for simplifying the theory of λ, they contain implicitly some optimistic assumptions about simplifying the theory of phonon dispersion. We confirm the conclusion of CDM[10] about the lack of correspondence between χ_1 and ω_Q. However, our work suggests that if the matrix element $\bar{M}_Q$ were properly included, a strong correspondence should appear between $\Pi_L(\vec{Q})$ and ω_Q. In other words, the anomalous structure seen in the phonon dispersion of these materials should be closely related to the part of $\Pi_1(\vec{Q}, 0)$ which arises from transitions within $\pm\hbar\bar{\omega} \simeq 0.022$ Ry of ϵ_F. This supports the finding of

Gupta and Freeman[21] for NbC and TaC that $\chi(q)$ has structure which correlates with ω_Q coming from *intra*-band transitions, while the much larger values coming from interband transitions are slowly varying with $\vec{Q}$. It remains mysterious why the neglect of matrix elements should destroy the correspondence between ω_Q and χ in Nb but not in NbC.

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