made an analogous, but less generalized calculation for the anisotropy of intraband warm carrier absorption. We refer to this paper for some additional mathematical details. It is important to note that for intraband absorption (a) the transition probability is different ($\propto \cos^2\theta$), and (b) the transitions are not direct, and hence the absorption coefficient reflects average rather than detailed features of the distribution function.

[8]The derivation in reference 7 for unpolarized light is in error.

[9]For $G_2/G_0 \lesssim 1$ as in all our measurements, it is a reasonable approximation to use $\alpha_E{}^0(\lambda) \approx \alpha_E(\lambda) \approx \alpha_E(\lambda)_{\text{unp}}$ for determining G_0.

[10]Using this relation, reasonable, although only approximate, values of ϵ as a function of λ are obtained for heavy holes, but not for light holes. The difficulties are due to warping of the bands and broadening effects. The latter, ascribed to the very short lifetimes of holes excited to the split-off band, are discussed by T. P. McLean and E. G. S. Paige, J. Phys. Chem. Solids 23, 822 (1962); Proceedings of the International Conference on Physics of Semiconductors, Exeter, 1962 (The Institute of Physics, University of Reading, Berkshire, England, 1963). As a consequence, the distribution functions can be analyzed only for the heavy holes, and even here with limited resolution.

[11]The rapid variation of G_2/G_0 with $\alpha_\parallel/\alpha_\perp$ [Eq. (5)] greatly enhances the scatter in the G_2/G_0 data. The ratio $\alpha_\parallel/\alpha_\perp$ was particularly difficult to obtain accurately at the higher carrier energies where both the zero-field absorption coefficient and the change in absorption are quite small.

[12]For additional details see references 1 and 2. In the former there is a discussion of the dependence of the energy distribution function on carrier concentration. In the present experiment we find within experimental error the same distributions for 5.9×10^{14} and 1.9×10^{15} holes/cm^3, for equivalent power input.

[13]For these calculations the scattering parameters for the interactions were taken from the zero-field mobility analysis of D. M. Brown and R. Bray, Phys. Rev. 127, 1593 (1962).

[14]A similar conclusion is reached by Brown, Paige, and Simcox, loc. cit, from measurements restricted to low field strengths, $E \leq 350$ V/cm.

[15]See, e.g., S. Chapman and T. G. Cowling, The Mathematical Theory of Nonuniform Gases (University Press, Cambridge, 1958), p. 347; E. M. Conwell, Phys. Rev. 88, 1379 (1952); G. G. Reik and H. Risken, Phys. Rev. 124, 777 (1961), which also contains many previous references.

LATTICE DYNAMICS OF NIOBIUM

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(Received 26 July 1963)

The frequency/wave-vector dispersion relation $\nu(\vec{q})$ for symmetry directions in niobium has been measured at 296°K by means of inelastic neutron scattering. The measured curves show certain unusual features which have not been observed previously. Analysis of the data on the basis of the Born–von Kármán theory indicates that the effective interatomic forces are of very long range; the actual forces in the metal are therefore extremely complicated. The Born–von Kármán force model has been used to calculate the frequency distribution function $g(\nu)$. It is of interest to compare this $g(\nu)$ with that for vanadium, already measured[1-5] using incoherent neutron scattering.

Except for iron,[6] very little work on the dispersion relations for transition metals has been attempted. The intriguing differences in the superconducting properties of the transition elements[7] in the fifth and sixth columns of the periodic table make this group of elements particularly interesting. The experiments and their interpretation are made easier by the fact that these elements have the same crystal structure, body-centered cubic. The incomplete d-electronic shells make an important contribution to the extremely large cohesive energies of these metals,[8] and it is likely that they also have a marked effect on the $\nu(\vec{q})$ dispersion relations. Niobium was chosen for initial study since its superconducting transition temperature is very high (~9.1°K), and the effects of a correspondingly large electron-phonon interaction might be apparent in the dispersion curves. Furthermore, its neutron scattering properties are very favorable.

The results of the measurements, most of which were made using the Chalk River triple-axis spectrometer in its constant-$\vec{Q}$ mode of operation,[9] are shown in Fig. 1 along the symmetry lines $[00\zeta]$, $[\zeta\zeta 0]$, $[\zeta\zeta\zeta]$, $[\frac{1}{2}\frac{1}{2}\zeta]$, and $[\zeta\zeta 1]$. Measurements were made with either the $(1\bar{1}0)$ or the (001) plane of the specimen horizontal. The initial slopes of the dispersion curves are in good agreement with those calculated from the measured elastic constants.[10] The following features of

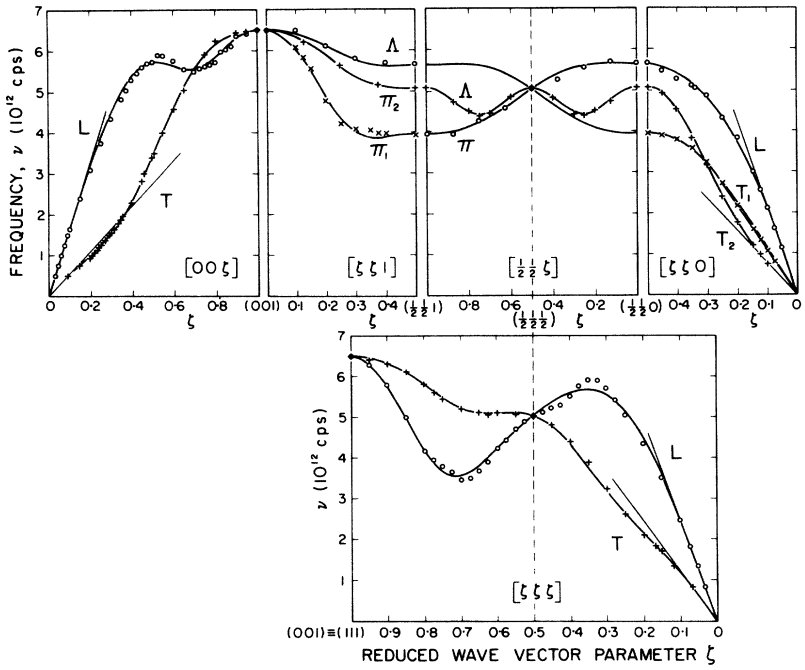

FIG. 1. The dispersion curves for niobium at 296°K for lattice waves traveling in the [00ζ], [ζζ0], [ζζζ], [ζζ1], [½½ζ] symmetric directions. The solid curves are the eighth-neighbor Born–von Kármán force-model least-squares fit.

particular interest are to be noted:

(1) The [00ζ] longitudinal (L) and transverse (T) branches cross at $\zeta \approx 0.7$. This crossing over of the acoustical branches in the absence of a symmetry requirement for this behavior has not been reported for any other material.

(2) The two nondegenerate [ζζ0]T branches (designated by T_1 and T_2, respectively) intersect at $\zeta \approx 0.3$.

(3) There occur an extra maximum and minimum in the [00ζ]L branch leading to two extra critical points in the frequency distribution.

(4) There is an increase in the value of $d\nu/d\zeta$ which occurs at about halfway across the zone for the [00ζ]T and [ζζ0]T_2 branches.

(5) There is a decrease below the elastic constants line for [00ζ]T near $\zeta = 0.2$. This represents a significant departure from the Debye spectrum at frequencies which are $\sim\frac{1}{7}$ of the maximum frequency for the crystal.

(6) Anomalies occur such as that in the [ζζζ]L branch at $\zeta \approx 0.45$ and the pronounced changes in slope at $\zeta \approx 0.47$ and $\zeta = 0.72$ for the [ζζζ]T branch.

Not unexpectedly, the analysis of these results on the basis of the Born–von Kármán theory required very long-range forces in order to fit the data. Fourier series analysis[11] indicated that forces out to at least tenth neighbors were important. A detailed fit for forces out to and including eighth neighbors was carried out using a Bendix G-20 computer. The results of this fitting process are also shown in Fig. 1 and Table I. It describes most of the features satisfactorily except for the behavior near (0.45, 0.45, 0.45)L.

The question of the physical significance of these long-range forces in metals is an important one and cannot be discussed properly without an adequate description of the effects of the electron-phonon interaction. Some of the unusual features mentioned above may be attributed to the Kohn effect[12] which has been observed in lead.[13] The treatment of the electron-phonon interaction, however, will be complicated by the existence of incomplete d shells. The Born–von Kármán fit with long-range forces serves a useful purpose since it may well provide some insight into this problem. For example, the Kohn effect shows up (theoretically) as an infinitely long-range force.

Another useful result of this detailed analysis based on the Born–von Kármán theory is the interpolation formula which can be used to calculate (with reasonable accuracy) the frequency of any other mode in the lattice; it is then straightforward to calculate the frequency distribution function, $g(\nu)$. This has been done using the eighth-neighbor model by calculating frequencies at

Table I. Force constants determined by the least-squares fit to the eighth-neighbor Born–von Kármán general force model (in units of 10 dyn/cm). The force-constant notation is similar to that of Woods.[a]

Position of neighbors	Force constants
$\frac{1}{2}a(1,1,1)$	$\alpha_1 = 1414 \pm 9$
	$\beta_1 = 884 \pm 12$
$\frac{1}{2}a(2,0,0)$	$\alpha_2 = 1416 \pm 9$
	$\beta_2 = -364 \pm 20$
$\frac{1}{2}a(2,2,0)$	$\alpha_3 = 227 \pm 7$
	$\beta_3 = -638 \pm 11$
	$\gamma_3 = 76 \pm 13$
$\frac{1}{2}a(3,1,1)$	$\alpha_4 = 361 \pm 9$
	$\beta_4 = -75 \pm 6$
	$\gamma_4 = -95 \pm 8$
	$\delta_4 = 126 \pm 5$
$\frac{1}{2}a(2,2,2)$	$\alpha_5 = -116 \pm 6$
	$\beta_5 = -133 \pm 12$
$\frac{1}{2}a(4,0,0)$	$\alpha_6 = -708 \pm 25$
	$\beta_6 = 132 \pm 14$
$\frac{1}{2}a(1,3,3)$	$\alpha_7 = -3 \pm 8$
	$\beta_7 = -10 \pm 5$
	$\gamma_7 = 37 \pm 8$
	$\delta_7 = -17 \pm 5$
$\frac{1}{2}a(4,2,0)$	$\alpha_8 = 51 \pm 6$
	$\beta_8 = -27 \pm 11$
	$\gamma_8 = 81 \pm 9$
	$\delta_8 = -6 \pm 7$

[a]A. D. B. Woods, Inelastic Scattering of Neutrons in Solids and Liquids (International Atomic Energy Agency, Vienna, 1963), Vol. II, p. 1.

45 526 independent positions in the irreducible sector of the ($\frac{1}{48}$) Brillouin zone, leading to a total of 6×10^6 modes in the full zone. The resultant frequency distribution is shown in Fig. 2(a). Figure 2(b) shows $g(\nu)/\nu^2$ [for $\nu < 1.25\times10^{12}$ cps, calculations of $g(\nu)/\nu^2$ were made on a finer mesh in order to obtain better statistics]. The deviation from a Debye spectrum is apparent at $\nu \approx 1\times10^{12}$ cps, a result which has already been anticipated from inspection of the dispersion curves.

In view of the similarities in the electronic structures (incomplete d shells and same number of valence electrons), it is perhaps reasonable to expect that these results for niobium bear some resemblance to the other transition metals in the same column, tantalum and vanadium. The frequency distribution function for vanadium has been measured directly using incoherent inelastic neutron scattering,[1-5] and several apparent anomalies have been observed.

Turberfield and Egelstaff[3] have reported a high-frequency tail in their results. The calculated $g(\nu)$ for niobium does have a pronounced shoulder near $\nu = 6.4\times10^{12}$ cps, but there is no evidence for a high-frequency tail. It is not impossible that this is only a reflection of the inadequacy of the eighth-neighbor model, however, since it is clear from Fig. 1 that it is not a perfect fit to the data, and, of course, only symmetry modes have been used in the fit. Nevertheless, this is considered unlikely.

Pelah et al. have reported[14] a low-energy hump in their measured $g(\nu)$ at $\nu \approx 2\times10^{12}$ cps which they attribute to a Kohn anomaly.[15] As noted above, it is quite possible that both niobium and vanadium are favorable cases for the observation of the Kohn effect. However, in this case, the argument for the assignment of the anomalous observed intensity at $\nu \approx 2\times10^{12}$ cps to the Kohn effect rests heavily on the premise that frequencies in these metals which are $\lesssim 0.3\nu_{\max}$ ($\nu_{\max} \sim 7\times10^{12}$ cps) should be accurately described by the Debye approximation, and therefore any departure from the Debye approximation is likely to be due to some anomalous effect, such as the Kohn effect.[15] It may be that the change in slope of $\nu(\tilde{q})$ for $[00\zeta]T$ near $\zeta \approx 0.15$, $\nu \approx 0.8\times10^{12}$ cps, is, in fact, a Kohn anomaly. On the other hand, the peak in $g(\nu)$ at $\nu \approx 1.2\times10^{12}$ cps (which looks similar to that observed by Pelah et al. in vanadium[14]) does not result from any specific anomaly at this frequency. It should be noted that this feature of $g(\nu)$ [and the corresponding behavior of $\nu(\tilde{q})$] are reproduced even when the experimental data for high-frequency modes ($\nu > 3\times10^{12}$ cps) and the elastic constants[10] only are used in the fitting process for the eighth-neighbor Born–von Kármán model.

These results show that the lattice dynamics of at least some of the transition elements are characterized by abnormal features which have not been observed in other metals. It is likely that the effects of the d electrons are very important in the interpretation of the lattice dynamics of transition metals, and calculations of the electronic structures of these metals may well show a correlation with these results. It is hoped to study other body-centered cubic transition metals in this series to see if any significant pattern emerges.

The authors would like to thank Dr. B. N. Brockhouse and Dr. G. Dolling for useful discussions. Mr. A. L. Bell, Mr. E. A. Glaser, and Mr. R.

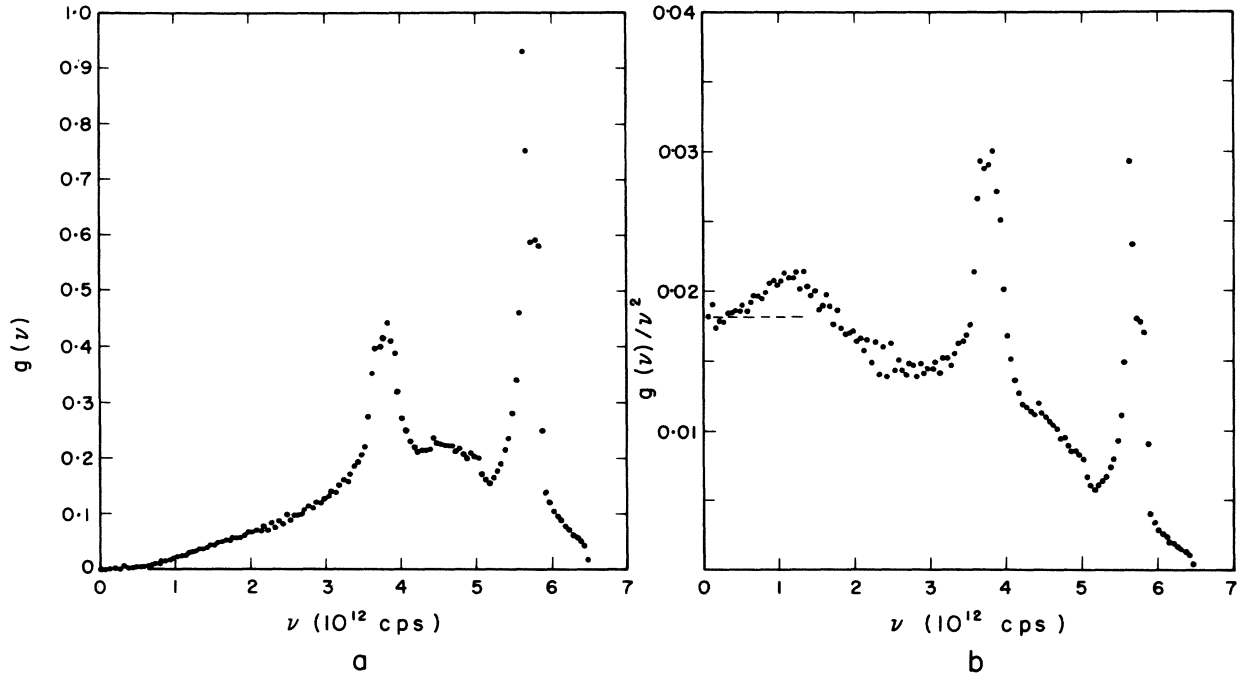

FIG. 2. (a) The frequency distribution function, $g(\nu)$, for niobium determined from the eighth-neighbor Born–von Kármán fit to the symmetry direction $\nu(\tilde{q})$ data. (b) $g(\nu)/\nu^2$, showing the departure from the Debye spectrum [$g(\nu) \propto \nu^2$] at low frequencies.

Rea gave valuable technical assistance.

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