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[4]E. F. Gross, N. V. Starostin, and R. I. Shekhmamet'ev, Fiz. Tverd. Tela 13, 3393 (1971) [Sov. Phys. Solid State 13, 2850 (1972)], claim to have observed M_3 electrons. Their interpretation of their data is subject to some criticism.

[5]R. J. Elliott, Phys. Rev. 108, 1384 (1957).

[6]$\epsilon_2(\omega)$ differs from the optical absorption coefficient by a factor that, in a limited region of the spectrum, may be taken to be constant. See J. D. Dow and D. Redfield, Phys. Rev. B 1, 3358 (1970), for explanation of notation.

[7]The Hulthén potential is discussed in A. G. Sitenko, *Lectures in Scattering Theory* (Pergamon, New York, 1971).

[8]In the static (linearized) self-consistent-field approximation we have (for zero temperature) $k_s^2 = 4\pi ne^2/\epsilon_0\mu_F$, where n is the number density of electrons and μ_F is the Fermi energy. Hence k_s is proportional to $n^{1/6}$.

[9]B. Velicky and J. Sak, Phys. Status Solidi 16, 147 (1966).

[10]Band-structure calculations indicate that distinct M_3-type structures are rarely prominent in the density of states over energies as much as 1 eV.

[11]This is unlikely. M_3 critical points generally occur (i) near the Brillouin zone boundary where the bands tend to be flat (heavy mass) as they meet periodic boundary conditions; or (ii) near the zone center in which cases their masses are often well estimated using nearly free-electron theory.

[12]Here m_1 is the band mass of the electron states (usually the lowest conduction band) determining the screening.

[13]M. Tanenbaum and H. B. Briggs, Phys. Rev. 91, 1561 (1953); E. Burstein, Phys. Rev. 93, 632 (1954).

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Experimental Evidence of Breakdown of Simple Pseudopotential Theory for Lattice Dynamics of Beryllium

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We present dispersion curves for phonons along ΓKM in Be. It is shown that the ordering of the branches corresponding to the phonon modes polarized in the basal plane at the symmetry point K provides a simple and direct qualitative criterion for the presence of tensor forces. The existing pseudopotential calculations of the dynamics are inherently incapable of explaining these results. Generalizations required in the theory are mentioned.

Measurements of phonon dispersion curves have been performed on a number of hexagonal close-packed metals,[1-4] and most of these data have been successfully explained on the basis of pseudopotential theory.[5-7] We present here new experimental results along ΓK in Be and show that the observed sequence and the degeneracy of the phonon branches at the point K cannot be reproduced *even qualitatively* within the framework of these calculations, and hence provide simple and direct evidence of the breakdown of simple pseudopotential theory in beryllium. We shall discuss the significance of this observation in relation to various theories of lattice dynamics.

The dispersion curves along ΓK were measured using a filter detector spectrometer.[8] Out of the six branches measured, four which are elliptically polarized in the basal plane are shown in Fig.

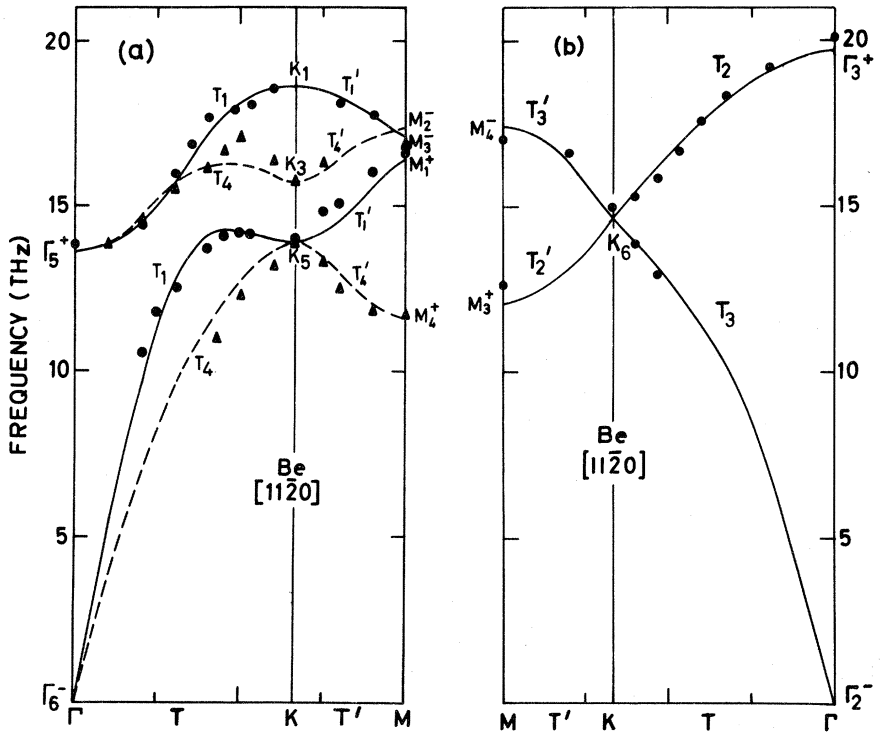

FIG. 1. Measured phonon dispersion curves in beryllium along ΓKM: (a) modes polarized in the basal plane, and (b) modes polarized perpendicular to the basal plane. The solid and dashed lines represent a six-neighbor force-constant model fit to the experimental results along ΓA, ΓM (Ref. 3), and ΓKM.

1(a); the remaining two, which have their polarization vectors perpendicular to the basal plane, are shown in Fig. 1(b). The branches have been labeled according to the group-theoretic notations.[9]

Symmetry demands that one of the T_1 branches [Fig. 1(a)] be degenerate with one of T_4 at the point K. For example, in magnesium[1] the acoustic T_1 branch is degenerate with the optic T_4, with one branch below this set and the other above. In beryllium, however, the acoustic T_1 and T_4 branches are degenerate, and the optic branches are well above as shown in the figure. It is this ordering which is of special interest to us, and therefore we write down the general expressions for these frequencies at K:

$$4\pi^2 M\nu_{K_5}{}^2 = D_{xx}(\vec{q}, 11) + \mathrm{Im}[D_{xy}(\vec{q}, 11)],$$

doubly degenerate,

$$4\pi^2 M\nu_{K_1}{}^2 = D_{xx}(\vec{q}, 11) + 2\,\mathrm{Re}D_{xx}(\vec{q}, 12) - \mathrm{Im}[D_{xy}(\vec{q}, 11)],$$

$$4\pi^2 M\nu_{K_3}{}^2 = D_{xx}(\vec{q}, 11) - 2\,\mathrm{Re}D_{xx}(\vec{q}, 12) - \mathrm{Im}[D_{xy}(\vec{q}, 11)],$$

where $D_{\alpha\beta}(\vec{q}, kk')$ denotes the dynamical matrix element.[10] The labeling of the branches at K according to the irreducible representations K_1, K_3, and K_5 are indicated in the figure.

It is clear from the above equations that in *any* theory in which $\mathrm{Im}[D_{xy}(\vec{q}, 11)]$ is zero, one frequency will be above and the other below the degenerate branch, in contrast to the experimental results in beryllium.

On the basis of a simple pseudopotential theory, microscopic calculations of dispersion curves without any adjustable parameters were first carried out in beryllium by Sahni and Venkataraman[11] using a local pseudopotential and a scalar dielectric function. These calculations did not give good agreement with the experiments along ΓA and ΓM. More sophisticated calculations based on Harrison's nonlocal theory[12] have been made by Gilat, Rizzi, and Cubiotti,[5] and King and Cutler,[6] who also have used a scalar dielectric function. The latter authors obtain good agreement with the measurements of Schmunk[2] along ΓA and ΓM. Similarly, Sahni and Venkataraman[11] have also obtained excellent agreement using a parametrized[13] *local* pseudopotential. However, in all these calculations,[5,6,11] which employ second-

order perturbation theory in the pseudopotential, starting with plane waves, only pairwise interactions are involved,[14] leading to a real $D_{xy}(\vec{q}, 11)$. Thus it is impossible to explain the ΓKM results, in particular the sequence of the branches at K in Be.

Since any calculation of phonon dispersion curves based on Harrison's nonlocal approach can be reproduced by using an "effective" local pseudopotential, it is of interest to consider a more general nonlocal pseudopotential formulation as given by Sinha and Gupta.[15] In this approach, which is based on the Born-Oppenheimer perturbation theory applied to actual conduction-electron wave functions, the pseudopotential occuring in the electron-phonon matrix element is split into a local and a nonlocal part. The latter part has a nonvanishing contribution to the dynamical matrix if the electron wave functions are not plane waves. Further, this contribution cannot be reduced to an axially symmetric form,[16] and it therefore implies the presence of non-pairwise forces which are essential for explaining the present results.

As an extension of the simple pseudopotential theory, Brovman and Kagan[17] have also shown that corrections in the dynamical matrix, arising from higher than second-order scattering of conduction electrons by a local pseudopotential, will give rise to tensor forces. Alternatively, in all the theories,[12,15,17] use of a nondiagonal screening function will also introduce non axially symmetric forces. However, for a non transition metal like beryllium, the free-electron scalar dielectric function with the proper inclusion of exchange and correlation effects may still be adequate.

Since the ordering at K is a direct consequence of the existence of tensor forces, it is of some interest to do a generalized tensor-force-constant analysis. By limiting interactions up to the sixth neighbors, it is found that the tensor-force interaction for the first neighbors in the basal plane alone[18] enters into the expression for $\mathrm{Im}[D_{xy}(\vec{q}, 11)]$. Using modified axially symmetric[19] interactions for the remaining neighbors, it is possible to fit the experimental[3] dispersion curves along ΓA, ΓM, and ΓK, to within 30%. The value of the tensor force constant δ (in the notation of Ref. 10), which is identically zero in a modified axially symmetric model calculation, is about 37% of the bond-stretching force constant[10] $(\alpha + 2\beta)$.

Coming to the other hcp metals we note that in magnesium[1] the sequence of the branches at K is consistent with the assumption of pairwise forces. In zinc, the sequence is qualitatively similar to that in magnesium, but there is a departure from the axially symmetric conditions,[4] and further there is other evidence[16] to suggest that the nonlocal character of the pseudopotential is important in zinc. For terbium[20] and holmium[21] the ordering of the branches at K[22] is similar to that in beryllium. For these rare-earth transition metals, in addition to nonlocality, the off-diagonal terms of the dielectric matrix will play an important part in determining the phonon spectrum.

To summarize, we have shown that the ordering of the phonon dispersion curves in beryllium at the point K is a direct manifestation of the existence of tensor forces, and hence cannot be explained on the basis of a simple pseudopotential theory.

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Shallow-Donor Negative Ions and Spin-Polarized Electron Transport in Silicon*

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Electron capture by neutral shallow donors is shown to be the dominant capture mechanism in uncompensated silicon at low temperatures. The mechanism is strongly dependent on spin polarization, which permits its separation from other competing mechanisms and the evaluation of its capture cross section. We also determine the negative donor-ion thermal ionization energy and lifetime.

A conclusive demonstration is presented that neutral donor capture, resulting in formation of the negative donor ion D^-, is the dominant electron capture mechanism in n-type silicon samples of sufficiently low compensation in the liquid-helium temperature region. The capture-rate constant (and cross section) of this process, the lifetime of the D^- ion against recombination with D^+ ions, and the thermal ionization energy of the D^- ion are determined for phosphorus, arsenic, and antimony donors. Separation of the contribution of D^0 electron capture from that of the D^+ "giant trap"[1] electron capture is effected by optically neutralizing the D^+ impurities with intrinsic radiation,[2] as well as by producing conduction and bound electrons of high spin polarization $\mathcal{P}$, to reduce the D^0 capture-rate constant.[3] The polarization dependence of the photocurrent which was formerly attributed to the mobility dependence associated with neutral impurity scattering[4,5] in silicon of intermediate donor and low acceptor concentrations is shown to be due primarily to the D^0 capture mechanism, as in the case of low donor concentrations.[3] The negative-donor-ion concentration $N(D^-)$ can be made comparable to or higher than the compensating impurity concentration, at modest illumination levels, and intrinsic illumination can thus strongly affect the charged impurity concentrations in a manner similar to that reported with intrinsic radiation.[2] The determination that the polarization dependence of the photocurrent arises primarily from D^0 capture rather than from neutral impurity scattering was implemented through the use of high magnetic fields up to 107 kOe, which permitted high polarizations to be attained over the entire liquid-helium temperature range. Hall-effect measurements in the polarized and unpolarized states confirm the conclusion. The reason that the neutral-impurity scattering mobility exhibits a much smaller $\mathcal{P}$ dependence than predicted by the simple scaled theory[4] is not completely clear, but a plausible explanation is proposed.

In Fig. 1 is shown the extrinsic photocurrent as a function of temperature for a phosphorus-doped silicon sample with low boron compensation [$N(P) = 9.5\times10^{15}$ cm^{-3}, $N(B) = 4.2\times10^{12}$ cm^{-3}].[6] The currents were measured in a magnetic field of 35 kOe, and the squares and circles refer, respectively, to equilibrium $\mathcal{P}$ values $\mathcal{P}_0$ and $\mathcal{P}=0$, with the latter condition obtained by resonating the Zeeman levels[5] of the neutral donors with 98-GHz low-power microwave radiation. $\mathcal{P}_0$ ranges from 0.9998 at the lowest temperature of our experiment (0.5 K) to 0.53 at $T = 4.0$ K. Extrinsic photocurrent is produced by a blackbody source at temperature $T_{BB} = 80$ K, reflected off a CaF_2 mirror in an arrangement similar to that de-