For α-Fe_2O_3 no measurement of the piezomagnetism exists in the literature, but we can deduce from a recent experiment[5] on the closely related linear magnetostriction of α-Fe_2O_3 that the piezomagnetic constants are on the order of 10^{-5}. For CoF_2 the measured values[6] are 2.1×10^{-3} and 0.8×10^{-3}, respectively. Our calculations suggest that the piezomagnetism of CoF_2 can be accounted for primarily by the strain dependence of the g tensor. Moriya[7] has given a calculation for P_{36} in which he neglects the "g" term in favor of the crystal-field splitting of the lowest lying quartet. Recent measurements[8] of the actual size of the crystal-field splitting of the ground quartet of Co^{2+} in MgF_2 and ZnF_2 show that his theoretical estimate greatly overemphasizes this effect.

We conclude that, to within the factor-of-2 type of error we expect on our model,[2,3] we may successfully predict piezomagnetism from epr under pressure and also shed light on the microscopic mechanisms involved in piezomagnetism.

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MODEL POTENTIALS AND THE DISPERSION LAW IN SOLID KRYPTON

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In an important experiment, Daniels *et al.*[1] have recently presented measurements on the dispersion of phonons in solid Kr at 3 bar and 79°K along the three principal symmetry directions. It is of considerable interest to see how well model potentials, such as the Lennard-Jones potential, can account for the results. Calculations of the dispersion law in solid Kr using the Lennard-Jones potentials were first carried out by Horton and Leech.[2] These calculations were done at 1 bar and 0°K, and so a comparison with the experimental results requires allowance for anharmonic effects. Calculations of these effects have been based on special models.[3] For the purpose of this Letter we will assume that

$$\omega(\vec{f},j)=\omega^{\text{q.h.}}(\vec{f},j)+\Delta\omega^{V}(\vec{f},j)+\Delta\omega^{\text{anh}}(\vec{f},j),$$

with

$$\frac{\Delta\omega^{V}}{\omega}=-\gamma\frac{\Delta V}{V},$$

and

$$\frac{\Delta\omega^{\text{anh}}}{\omega}=\frac{A}{3Nk}E_{\text{vib}},$$

$$E_{\text{vib}}=kT\sum_{\vec{f},j}\left[\frac{1}{2}x+\frac{x}{e^{x}-1}\right],\quad x=\frac{\hbar\omega(\vec{f},j)}{kT}.$$

$\gamma=2.9$ is an average Grüneisen parameter assumed to be independent[4] of $(\vec{f},j)$. $\omega^{\text{q.h.}}(\vec{f},j)$ refers to frequencies obtained from a harmonic dynamical matrix in which the effect of the zero-point energy is included via the potential parameters.[2] The assumption that the anharmonic frequency shifts can be represented as above,[5] with A independent of $(\vec{f},j)$, is used here as a reasonable first approximation. The value of $A\approx1\times10^{-3}/°K$ has recently been calculated for Lennard-Jones potentials.[6] (For our purpose, we can also ignore the model dependence of A.) Since the crystal of Kr in the pressure vessel was measured to have a

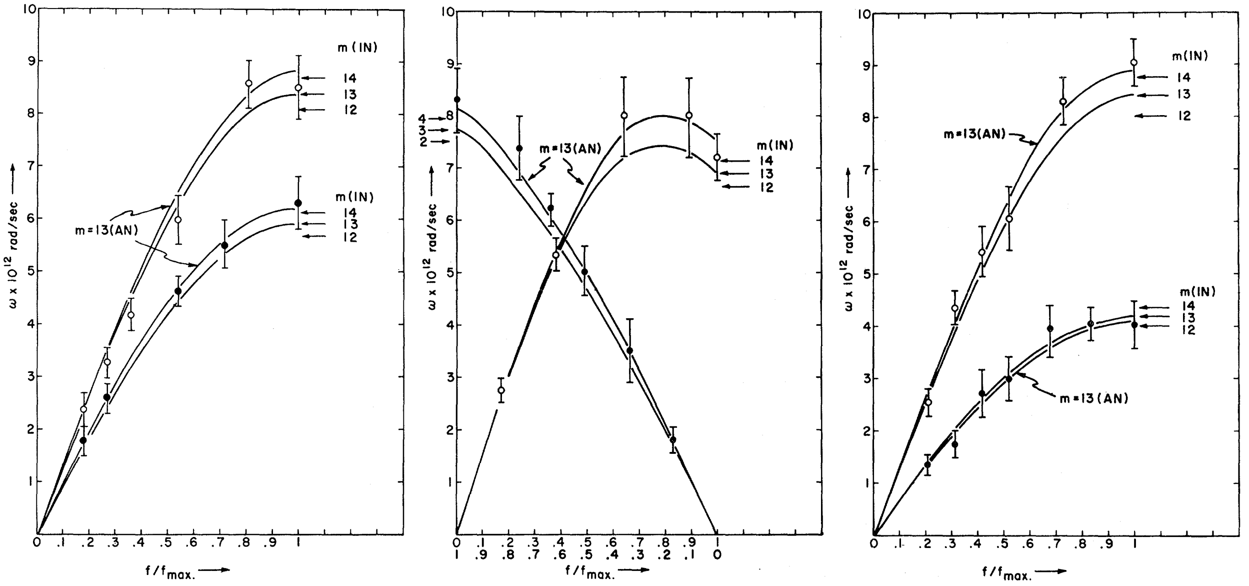

FIG. 1. The phonon dispersion law in the [100], [110], and [111] directions in solid Kr at ~73°K and 1 bar. The data are due to Daniels et al.[1]; the theoretical curves, based on an $(m-6)$ Lennard-Jones potential, are taken from Horton and Leech[2] and corrected approximately for anharmonic effects as described in the text. The experimental results for one of the transverse branches in the [110] direction are not available.

lattice parameter of 5.725 Å and the 0°K lattice parameter is known to be[7] 5.6458 Å, we conclude that

$$\omega(\vec{f},j) \approx 0.94\omega^{\text{q.h.}}(\vec{f},j).$$

The volume shift was about $-12\,\%$ and the anharmonic shift was about $+6\,\%$.

In Fig. 1 we present the results for the Lennard-Jones potentials

$$\varphi(r)=\frac{6m\epsilon}{m-6}\left[\frac{1}{m}\left(\frac{\sigma}{r}\right)^{m}-\frac{1}{6}\left(\frac{\sigma}{r}\right)^{6}\right],$$

using the parameter for Kr calculated by Horton and Leech.[2] No significant improvement in the fit is obtained by using Buckingham potentials.[8]

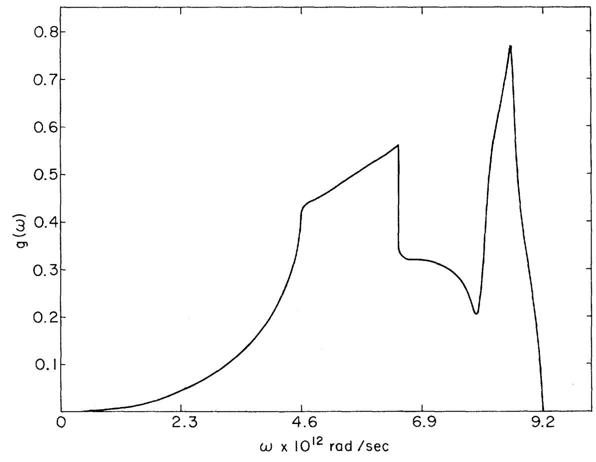

FIG. 2. The normal mode frequency distribution in solid Kr near $T = 0$°K at 1 bar. The function corresponds to a (14-6) (1N) model.

Our results show that an $m = 13$ all-neighbor (AN) and an $m = 14$ first-neighbor (1N) potential is compatible with the data of Daniels et al.[1] Using the method of Gilat and Raubenheimer[9] and the $m = 14$ (1N) model, we present in Fig. 2 the first approximation to the frequency distribution in solid Kr near $T = 0$°K.

We thank Dr. Daniels for communicating the experimental results to us before publication and for his hospitality to one of us (GKH). We acknowledge a useful discussion with Dr. T. H. Keil. This work was supported by the U. S. Air Force Office of Scientific Research under grant No. AFOSR 726.65. One of us (GKH) would like to thank the Rutgers Research Council for the award of a faculty fellowship.

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[4] The errors involved are at most ~10%; see D. C. Wallace, Phys. Rev. 139, A877 (1965).

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$$\varphi(r) = \frac{6n\epsilon}{n-6}\left[\frac{1}{n}e^{-n(r/\sigma-1)} - \frac{1}{6}\left(\frac{\sigma}{r}\right)^6\right];$$

for $n = 14$ (1N), the dispersion curves lie about 2% below the Lennard-Jones $m = 13$ (1N) case. $n = 15$ (1N) gives a reasonable fit.

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PHOTOEMISSION STUDY OF THE ELECTRONIC STRUCTURE OF CdTe†‡

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Cardona and Greenaway's identifications of the E_0', E_1', and $E_1'+\Delta_1$ peaks in the optical reflectivity spectrum of CdTe are contradicted by deductions drawn from photoemission measurements. New identifications of these peaks are proposed on the basis of these photoemission measurements and the results of empirically adjusted orthogonalized-plane-wave energy band calculations. Our theoretical band model for CdTe differs in some important respects from that derived by Cohen and Bergstresser using the empirical pseudopotential method.

The study of the band structure of semiconductors has been revolutionized by optical reflectivity measurements,[1] by the interpretation of optical spectra in terms of critical-point transitions,[2] by empirical energy-band calculations,[3-5] by electroreflectivity measurements,[6,7] and by piezoreflectivity measurements.[8] In view of the apparent success of the initial interpretations[2,3] of the optical spectra of Si and Ge, similar interpretations[9,10] have been made for a number of related materials, including III-V, II-VI, and even I-VII compounds. These interpretations form the basis of empirical (pseudopotential[3,4] and full-zone $\vec{k}\cdot\vec{p}$[5]) band calculations which are designed to support the interpretations upon which they are based. Interpretation of optical spectra and empirical band calculations form a closed cycle which can very easily perpetuate errors of interpretation and propagate such errors from one class of crystals to another. In order to discover and eliminate interpretational errors, it is essential to bring independent theoretical and experimental methods into play.

One of us (FH) has recently carried out an independent theoretical study[11] of the band structure of Si, Ge, and α-Sn which casts doubt on currently accepted interpretations[2-5,10] of the