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Deformation Potentials of the Alkali Halides*

Anibal Gavini† and T. Timusk
Department of Physics, McMaster University, Hamilton 16, *Ontario, Canada*
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The ratios of the shear deformation potentials b_{ex} and d_{ex} to the hydrostatic deformation potential a_{ex} of the first excitonic transition of KI, RbI, and CsI have been determined from piezoreflectance measurements. The obtained values do not agree with obtained values from piezobirefringence measurements of Gavini and Cardona. The difference is qualitatively explained in terms of the difference between the band-edge deformation potentials and the deformation potentials of the exciton.

The shear deformation potentials of the first excitonic transition of KI and KBr have been measured by Gerhardt and Mohler [1] using the piezoreflectance technique. More recently, the band-edge deformation potentials of a series of alkali halides have been obtained from piezobirefringence measurements. [2] The values obtained by these two methods differ in some cases by more than 100%; these differences are much larger than any error that can be attributed to the experimental techniques. In this paper, we reproduce Gerhardt-Mohler measurements in KI using a similar technique and extend these to RbI and CsI.

The piezoreflectance measurements were performed by stressing long thin single crystals using a PZT-4 transducer. [3] The stress was applied along the [100], [110], and [111] crystallographic directions. All measurements were performed at room temperature. Standard ac phase-sensitive techniques were used to obtain $\Delta\underline{R}/\underline{R}$.

Results for KI with the stress applied along the [110] direction and light polarized parallel and perpendicular to the direction of the stress are shown in Fig. 1. Similar measurements for CsI with the stress applied along the [111] direction are shown in Fig. 2. The results for RbI are similar to those for KI and will not be shown.

For all three materials, the measurements with the stress applied along the [100] direction show that the intensity of the signal is practically polarization independent, showing that the appropriate deformation potential is very small, in agreement with previous measurements. [1]

From the ratio of the intensity of the signal parallel and perpendicular to the direction of the stress, the ratio of the shear deformation potentials of the exciton b_{ex} and d_{ex} to the hydrostatic deformation potential a_{ex} can be obtained. [4] In Table I we show the values obtained for b_{ex}/a_{ex} from measurements performed with the stress applied along the [100] direction; also in the same table the values of d_{ex}/a_{ex} are given. These last values were obtained from measurements with the stress applied along the [110] direction in KI and RbI and along the [111] direction in CsI.

From the piezobirefringence measurements in the effective-mass approximation it is possible to obtain values for b and d, the shear deformation potentials of the band edge. These deformation potentials can be related to b_{ex} and d_{ex} under several assumptions. [5] However, in the light of the present results the validity of some of these assumptions can be questioned. The values obtained for b_{ex} and d_{ex} from the piezobirefringence experiments together with those obtained from the piezoreflectance measurements have been given in Table II for the sake of comparison. The large differences between the values obtained from the piezoreflectance and the piezobirefringence measurements are much larger than possible experimental error. However, these two techniques have been previously used in determining deformation potentials very successfully. [6–9] We have to conclude therefore that in these two experiments we are measuring different quantities.

There is no doubt that in the piezoreflectance measurements presented here we actually measure the deformation potentials of an isolated exciton in a very direct way (the binding energy of the exciton is three or four orders of magnitude larger than the stress-induced shifts). However, in the piezobirefringence measurements, the results will be affected by any states lying within 1 eV from the exciton (1 eV is approximately how near to the first exciton one can perform the piezobirefringence measurements at room temperature). Within this energy range we have several states: the spin-orbit split exciton, and the forbidden $J = 2$ and $J = 0$ excitons. Before stressing the crystal these last two states do not have any oscillator strength, but the externally applied stress will mix the $J = 2$ and the $J = 1$ states such that the former state may have an appreciable contribution to the piezobirefringence. However this $J = 2$ exciton will not be seen in the piezoreflectance measurements if the stress is much smaller

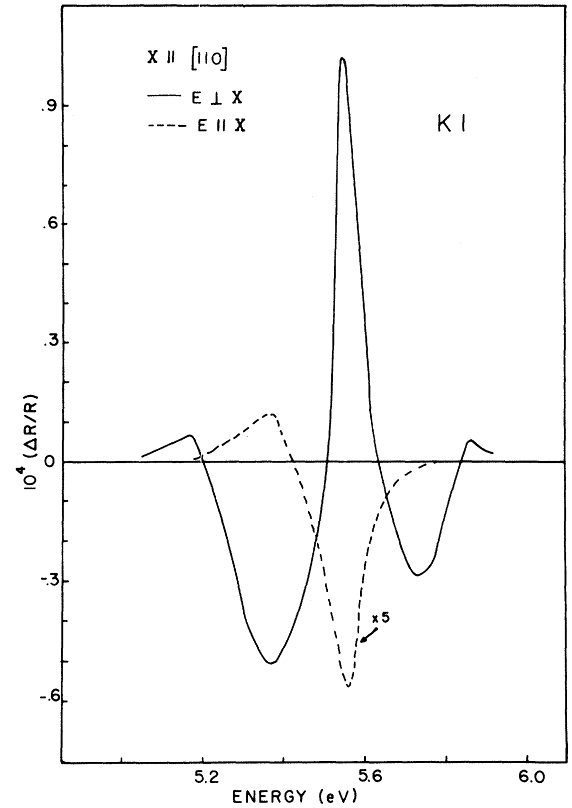

FIG. 1. Piezoreflectance spectra of KI for the stress applied along the [110] direction.

than in the piezobirefringence experiments, which is generally the case. It has also been shown that the stress may have a very appreciable effect in the magnitude of the spin-orbit splitting[10,11]; this effect was not considered in the interpretation of the piezobirefringence measurements.

It is obvious that all these effects have to be evaluated theoretically in order to relate the results of piezobirefringence to those of piezoreflectance. One can, however, say that while the piezoreflectance measures the deformation potentials of the Γ_{15} exciton, the piezobirefringence reflects "average" exciton deformation potentials, i.e., the deformation potentials of the hypothetical Γ_8-one-electron valence-band edge. Conservation of oscillator strength leads to the conclusion that exciton splittings should not affect the piezobirefringence at energies which differ from the exciton energies more than the excitonic splittings. Thus the good agreement between the "band" deforma-

TABLE I. Ratio of the shear deformation potentials b_{ex} and d_{ex} to the hydrostatic deformation potential a_{ex} obtained from the piezoreflectance measurements.

	b_{ex}/a_{ex}	d_{ex}/a_{ex}
KI	0.01 (±0.03)	−0.32 (±0.05)
RbI	0.03 (±0.03)	−0.31 (±0.05)
CsI	0.00 (±0.03)	+0.21 (±0.05)

TABLE II. Values of the deformation potentials b_{ex} and d_{ex} obtained from the piezoreflectance and piezobirefringence measurements.

	b_{ex}(eV)		d_{ex}(eV)	
	Piezoreflectance	Piezobirefringence (Ref. 2)	Piezoreflectance	Piezobirefringence (Ref. 2)
KI	0.08(Ref. 1) −0.03[a]	−0.22	0.55(Ref. 1) 0.73[a]	0.21
RbI	−0.09[a]	−0.23	0.72[a]	0.18
CsI	0.00[a]		−0.51[a]	−0.22
KBr		−0.40		0.17
RbBr		−0.40		0.15
CsBr		0.50		

[a] These measurements, the values for a_{ex} have been obtained from Ref. 1 for KI, D. W. Lynch and A. D. Brothers, Phys. Rev. Letters 21, 689 (1968) for CsI, and for RbI the same value as for KI has been used.

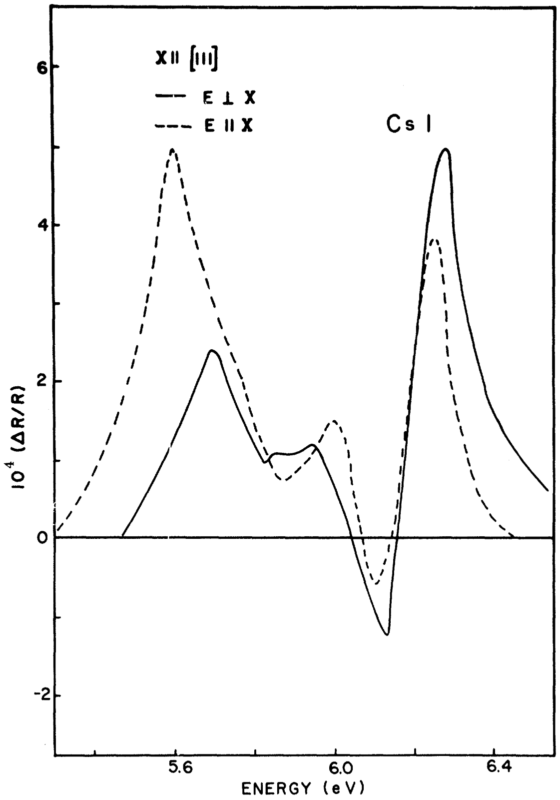

FIG. 2. Piezoreflectance spectra of CsI for the stress applied along the [111] direction.

tion potentials obtained from piezobirefringence and those calculated with the simple model that attributes the deformation potentials to the effect of the Madelung potential in the anisotropic "p" wave function of the valence band of the stressed crystal[2] is not surprising.

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[†] Present address: Superior Electronics, Inc., Montreal 331, Quebec, Canada.

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Pseudopotential Calculation of the Knight Shift and Relaxation Time in Magnesium

P. Jena* and T. P. Das*
Department of Physics, University of Utah, Salt Lake City, Utah 84112

and

S. D. Mahanti
Bell Telephone Laboratories, Murray Hill, New Jersey

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A nonlocal pseudopotential procedure has been utilized to obtain the conduction electron wave functions in magnesium metal. It is found that the use of these wave functions along with a finer scanning of the Fermi surface, namely, 110 points in $\frac{1}{24}$ of the Brillouin zone, leads to a value for the Knight shift K_s in much better agreement with experiment than was an earlier value obtained by the orthogonalized-plane-wave procedure. Possible sources for the difference in theoretical K_s values obtained by using these two different procedures are discussed. Improved values of the relaxation time T_1 and Korringa constant are also presented.

In a recent paper[1] we have analyzed the Knight shift (K_s) and nuclear spin-lattice relaxation time (T_1) in magnesium using wave functions obtained from orthogonalized-plane-wave (OPW) calculations. These calculations incorporated the effects of exchange core polarization[2] (ECP) and the exchange enhancement of spin susceptibility (χ_s) through currently available procedures.[3] The theoretical value of the Knight shift was[1] found to be 0.056% as compared to the experimental value[4,5] of 0.112%. In a search for possible sources for improving the agreement between experiment and theory, we have reevaluated the conduction electron spin density $\langle|\Psi_{\vec{k}_F}(0)|^2\rangle_{\mathrm{av}}$ using wave functions derived from available[6] nonlocal pseudopotential band calculations in this metal. In addition to the usefulness of such an analysis in explaining hyperfine properties of magnesium, the results are also useful in explaining the relationship between wave functions obtained by direct OPW calculations and through the use of pseudopotentials. Such a comparison is important in view of the increasing use that is being made currently of pseudopotentials and model potentials, not only for investigation of properties depending on the band structure, but also of hyperfine properties depending on wave functions. No such comparison is currently available for the hyperfine properties in any one metal. Magnesium[6,7] and indium[8,9] are the only two metals where such a comparison is currently possible due to the availability of both types of band calculations.

The nonlocal pseudopotential parameters utilized were those recently obtained by Kimball