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Experimental gradient elastic tensors: Measurement in I-VII semiconductors and the ionic contribution in III-V and I-VII compounds*

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Nuclear-acoustic-resonance measurements have determined the magnitudes and relative signs of the two nonzero tensor components, S_{11} and S_{44}, of the tensor S which relates elastic strain to electric field gradients at a nuclear position of ^{63}Cu^{35}Cl, ^{63}Cu^{79}Br, and ^{63}Cu^{127}I. The measured magnitudes of S_{11} in these I-VII compounds and in seven III-V compounds are shown to agree with calculated values of an ion-charge model based on free-atom values. Such agreement is found if ion charges characteristic of covalent bonding are used for the III-V compounds and ion charges characteristic of ionic bonding are used for I-VII compounds.

I. INTRODUCTION

Semiconducting crystals of the I-VII compounds of CuCl, CuBr, and CuI are expected to be among the most ionic crystals with the zinc-blende crystal structure according to the theories of Phillips[1] and Harrison.[2] It is therefore of great interest to be able to interpret the sources of electric field gradients at nuclear positions due to the chemical bonding when these crystals are externally strained. The tensor of the fourth rank S which relates the electric-field-gradient tensor V, to the elastic strain tensor ϵ at a nuclear position is defined by

$$V_{ij}=\sum_{k,l} S_{ijkl}\,\epsilon_{kl}\ . \tag{1}$$

In terms of the Voigt notation and with respect to engineering strains, the nonzero components of S for a crystal with local T_d tetrahedral symmetry are S_{11}, S_{12}, and S_{44}. With the assumption that the electric charge at the nuclear position does not change with strain,[3] $S_{11}=-2S_{12}$. In this paper, we report the nuclear-acoustic-resonance (NAR) determinations of S_{11} and S_{44} at the nuclear positions in ^{63}Cu^{35}Cl, ^{63}Cu^{79}Br, and Cu^{127}I and of S_{11} at ^{63}CuI. In addition, we point out an extension of the interpretation of S_{11} as only due to ionic contributions which has been developed in two earlier publications which we call I[4] and II.[5]

II. EXPERIMENTAL

As in the NAR experiments described in I, time-varying elastic strains due to acoustic waves produce time-varying electric field gradients at nuclear positions. When the nucleus possesses a nuclear electric quadrupole moment, acoustic energy may be coupled to the nuclear-spin system via the dynamic interaction of the quadrupole moment with these time-varying electric field gradients. This is the case for the nuclear positions in the I-VII semiconductors. The technique of NAR[6] measures the acoustic attenuation change associated with the absorption of resonant acoustic energy by the nuclear-spin system. In the S tensor measurements described in this paper, the nuclear-spin transitions involving the nuclear-spin quantum number m changing by 2 ($\Delta m=\pm 2$) were studied. The S tensor component S_{11} was determined by using transverse acoustic waves with a propagation vector $\vec{k}$ along [110] and polarization vector $\vec{\xi}$ along $[1\bar{1}0]$. Using the notation of I, we write

$$\Delta\alpha_{(\Delta m=\pm 2)}=\tfrac{9}{4}CB_2(QS_{11}\cos\chi)^2\ , \tag{2}$$

where χ is the angle in the $(1\bar{1}0)$ plane between $\vec{k}$ and the external field $\vec{H}$, and

$$C=\frac{\pi^2}{16(2I)^2(2I-1)^2(2I+1)}\,\frac{N\nu^2e^2g(\nu)}{\rho v^2kT}\ ,$$

$$B_2=\sum_m F_m(I)^2_{\pm 2}\ ,$$

$$F_m(I)_{\pm 2}=[(I\mp m-1)(I\mp m)(I\pm m+1)(I\pm m+2)]^{1/2}\ .$$

In the above expressions, I is the nuclear spin, N is the number of resonant nuclear spins per unit volume, ν is the elastic-wave frequency, $g(\nu)$ is the normalized line-shape function, ρ is the mass density, k is the Boltzman constant, v is the acoustic wave velocity, and T is the absolute temperature.

The S tensor component S_{44} was measured by propagating acoustic waves with $\vec{k}$ along [110], and $\vec{\xi}$ along [001]; ψ is the angle in the (001) plane between $\vec{k}$ and $\vec{H}$:

$$\Delta\alpha_{(\Delta m=\pm 2)}=4CB_2(QS_{44}\sin\psi)^2\ . \tag{3}$$

The relative signs between S_{11} and S_{44} were determined by propagating longitudinal waves with $\vec{k}$

along [110] and $\vec{H}$ in the (001) plane

$$\Delta\alpha_{(\Delta m=\pm 2)} = CB_2Q^2(\tfrac{3}{4}S_{11} - S_{44}\cos 2\psi)^2 \;. \tag{4}$$

Large single crystals of CuCl, CuBr, and CuI were grown by one of us (C.S.) using the traveling-solvent technique. The crystals were cut from rods to be approximate right cylinders. Two 1.3-cm-diam parallel (110) faces were ground approximately 1.3 cm apart. The end faces of the cylindrical samples were made flat and parallel to within 1.4 μm and were determined to be within 0.1 deg of (110) planes using x-ray diffraction techniques.

Acoustic waves were generated by means of *AT*-cut and *X*-cut quartz piezoelectric transducers bonded to the samples with solid phenyl-salicylate, "Salol." The coaxial cylindrical 10 MHz transducers are 1.27 cm in diameter with a center radiating diameter of 1.04 cm. Acoustic properties (mechanical resonance center resistance, shape, and frequency width) were measured using a Hewlett-Packard 250A RX meter. NAR absorption measurements were made at 10 MHz and 300 K utilizing a standard marginal oscillator ultrasonic spectrometer.[7] Absolute change in acoustic attenuation was determined by comparing the NAR absorption signal with a known calibrator signal.[8] The area under the absorption line shape was obtained by numerically integrating the experimentally observed NAR first derivative signal. Magnetic field modulation was used with modulation amplitudes chosen to be no larger than $\frac{1}{8}$ the peak to peak experimental line shapes. The dynamic strain amplitudes were chosen to produce less than 1% saturation of the NAR signal.

Because of the relative small values of the elastic constants c_{11}, c_{12}, and c_{44} in the three I-VII compounds, acoustic coupling even to the small quadrupole moment $\mathrm{Cu}^{35}\mathrm{Cl}$ nuclear-spin system could be observed with an NAR signal-to-noise ratio of $\frac{5}{1}$ for a single pass utilizing a noise bandwidth equivalent to an *RC* time constant of 30 sec. Signal averaging was used to improve all signal-to-noise ratios.

III. EXPERIMENTAL RESULTS

The basic coupling between elastic waves and the nuclear-spin systems in the I-VII compounds was verified to be via the nuclear electric quadrupole moment from (i) ability to observe both $\Delta m = \pm 1$ and $\Delta m = \pm 2$ NAR absorption lines and (ii) the measurement of the predicted angular dependences of the NAR absorption as given in Eqs. (2)-(4). The experimental line shapes in each of the three I-VII compounds were large compared to the predicted dipole-dipole widths and increased with regrinding of crystal faces and successive transducer bonding. The changes in width due to crystal handling indicate quadrupole broadening possibly due to increase in the number of internal strains. Because of relative poorer acoustic properties of CuI, it was impossible to measure the value of S_{44} for ^{35}CuI. The measured *g* values and relative signs of the values of S_{11} and S_{44} for the I-VII semiconductors are given in Table I.

IV. COMPARISON OF MEASURED S_{11} WITH THAT COMPUTED FROM AN ION CHARGE MODEL

As noted in I the electric-field-gradient tensor components can be written as the sum of ionic and electronic parts. If we choose *x*, *y*, and *z* to be the principal axes of the electric-field-gradient tensor then only diagonal components are different from zero. We also choose *x*, *y*, and *z* to lie along the cubic directions of the zinc-blende structure crystal. The ionic and electronic contributions to V_{zz} are given in the following equation:

$$V_{zz} = \sum_{i=1}^{4} \frac{(3\gamma_i^2 - 1)Z^*(1-\gamma_S)}{d^3} + \sum_{i=1}^{4} \frac{(-1)(3\gamma_i^2 - 1)}{2} \times 2e(1-R_S)\langle b_i | \frac{3\cos^2\theta_i - 1}{r_i^3} | b_i \rangle \;, \tag{5}$$

where γ_i is the direction cosine from the *z* principal axis to the *i*th bond direction, Z^* is the effective charge of the nearest-neighbor atom (including the sign of the charge), γ_S and R_S are the Sternheimer antishielding and shielding factors[9] for the solid, *d* is the nearest-neighbor distance, b_i is the total bond orbital wave function, and θ_i and r_i are the coordinates of the *i*th electron expressed with respect to an orthogonal coordinate system with its *z* axis along the *i*th bond direction. The factor

TABLE I. Measured values of S_{11} and S_{44} for I-VII semiconductors. S_{11} and S_{44} are in units of 10^{15} statcoulombs cm^{-3} and *Q* values are in units of 10^{-24} cm^2. Quadrupole moments are expressed with shielding corrections made. Experimental uncertainty of QS_{11} and QS_{44} is ±6% for ^{63}Cu and ^{35}Cl and ±4% for ^{79}Br and ^{127}I.

Nuclear position	Q	S_{44}	S_{11}
$\mathrm{Cu}^{35}\mathrm{Cl}$	0.09 ± 0.02[a,b]	±7.6	±7.9
$\mathrm{Cu}^{79}\mathrm{Br}$	0.29 ± 0.02[b,c]	±22.8	±14.7
$\mathrm{Cu}^{127}\mathrm{I}$	0.80 ± 0.05	±29.2	±22.6
$^{63}\mathrm{CuCl}$	0.21 ± 0.01[a,d]	±4.0	±6.6
$^{63}\mathrm{CuBr}$	0.21 ± 0.01[a,d]	±7.5	±4.5
$^{63}\mathrm{CuI}$	0.21 ± 0.01[a,d]		±4.7

[a] R. M. Sternheimer, Phys. Rev. 105, 158 (1957).

[b] C. H. Townes, *Handbuck der Physik* (Springer-Verlag, Berlin, 1958), Vol. 38, Pt. 1, p. 377.

[c] R. M. Sternheimer, Phys. Rev. 86, 376 (1952).

[d] D. Bleaney, K. D. Bowers, M. H. L. Pryce, Proc. R. Soc. A 228, 166 (1955).

$\frac{1}{2}(3\gamma_i^2 - 1)$ is due to the transformation of the electronic part from a coordinate system with its z axis along the ith bond direction to the z direction of the principal axes. The factor 2 in the electronic part come from assuming two electrons per bond, and the minus sign is from the field-gradient definition.[10]

The Sternheimer term $1-\gamma_s$ is introduced to correct V_{zz} at a nuclear position of an ion due to the interaction of the ion with its nuclear quadrupole moment and with the external point-charge electric field gradient. The term $1-R_s$ is a shielding correction to account for the shielding effect of the core electrons in the atom whose nucleus is the coordinate origin.

The first term in Eq. (5) is the ionic term written only for the first-neighbor shell. The second term is the electronic contribution. In I, we indicated, for atomic orbitals, that in the term $\langle b_i|(3\cos^2\Theta_i - 1)/r_i^3|b_i\rangle$, b_i could be replaced by the orbitals on the atom at whose nucleus V_{zz} is being computed. Other contributions to $\langle b_i|(3\cos^2\Theta_i - 1)/r_i^3|b_i\rangle$ were shown to be two orders of magnitude smaller.

For zero strain, we expect $V_{zz}=0$. With the expansion of Eq. (5) in a Taylor series in a particular component of strain, S_{11} and S_{44} can be identified as the components linear in strain. In order to relate the field gradient expression of Eq. (5) to the experimental strain, we choose V_{zz} to be along a [100] crystal direction and transform V_{ij} to a nonprincipal axis coordinate system with x' along [110], y' along [1$\bar{1}$0], and z' along [001]. We find S_{11} by expanding the $x'y'$ component of the transformed V_{ij} in a Taylor series in the shear strain $e_{x'y'}$. The $e_{x'y'}$ strain produces displacements which can be written in terms of their radial and angular contributions relative to the bond directions and the first-neighbor positions. From Fig. 1, we see that only angular displacements of the four first-neighbor bonds and four first-neighbor positions contribute to S_{11}. We note that in measuring S_{11} we have propagated the $e_{x'y'}$ strain wave with a sound wave velocity $v=[(c_{11}-c_{12})/2\rho]^{1/2}$.

Harrison and Phillips[11] have shown that good agreement is found between predicted bond-orbital-model values of the elastic constant $c_{11}-c_{12}$ and measured $c_{11}-c_{12}$ values when a particular bond displacement model is assumed. The assumed model is that the shear strain $e_{x'y'}$ does not alter the tetrahedral angles at either anion or cation in zinc-blende structure compounds, but that the bond to first-neighbor atoms is broken by the shear strain. The use of the Harrison and Phillips model with the strains which measure S_{11} leads to the conclusion as observed in II that the electronic contribution to S_{11} is zero: (i) the electronic part of S_{11} depends on angular changes in the orbitals of the atom at whose nucleus S_{11} is measured. (ii) the model of Harrison and Phillips predicts there are no angular changes in these orbitals.

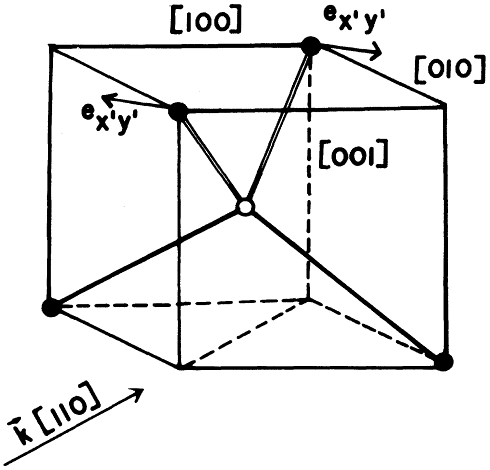

FIG. 1. First-neighbor shear-strain directions relative to a center atom at whose nucleus the electric field gradients are measured.

From the above argument, S_{11} has only ionic contributions and can be written

$$S_{11\,\text{ionic}} = \tfrac{16}{3} Z^*(1-\gamma_s)/d^3 \,. \tag{6}$$

In computing the $\frac{16}{3}$ term in Eq. (6), we do not know how the low-frequency dielectric function varies as a function of distance from the observing nuclear position. We therefore assume a dielectric step function which is one at the first-neighbor shell and the low-frequency dielectric constant for more distant shells. Such an assumption means that neighboring shells contribute only several percent of the first-neighbor shell and we approximate the total contribution by the first-neighbor shell contribution of $\frac{16}{3}$. In comparing Eq. (6) with experimental values of S_{11}, we, in addition, assume that $1-\gamma_s$ can be approximated by its free-atom value $1-\gamma_\infty$ and require a value of Z^* to bring agreement between $S_{11\,\text{ionic}}$ and the measured S_{11}. We call the above assumptions used in estimating the magnitude of $S_{11\,\text{ionic}}$ in Eq. (6) the "ion-charge model."

A. III-V compounds

The two basic types of chemical bonding in the III-V compounds[12] such as AlSb are (i) covalent or homopolar with three electrons from Al and five from Sb creating the electronic bond and leaving ion cores of Al^{3+} and Sb^{5+} and (ii) ionic or heterpolar with Al losing all its valence electrons to Sb so that both atoms have closed electron shells and are ions Al^{3+} and Sb^{3-}. The actual chemical bonding[12] is believed to lie between these two extremes. The ions in homopolar bonding are expected to be par-

TABLE II. Comparison of the required first-neighbor charge Z^*/e at Sb in AlSb to produce agreement with the experimental S_{11} at the Al nuclear position for different Al ionic states. S_{11} and $16e/3d^3$ are in units of 10^{15} statcoulomb cm^{-3}.

Ion	$(1-\gamma_\infty)^{a}$	$\frac{16}{3}e/d^3$	$S_{11}{}^{b}$	$Z^*/e=S_{11}/(1-\gamma_\infty)$ $(16e/3d^3)$
Al^{1+}	2.27	0.1366	2.6	8.4
Al^{2+}	2.79	0.1366	2.6	6.8
Al^{3+}	3.30	0.1366	2.6	5.8

[a] See Ref. 13. [b] See Ref. 4.

tially shielded by the two electrons in each of four bonds between a center atom and its four first neighbors resulting in an effective lattice charge[2] Z^* associated with each of the four first-neighbor atoms. We note that the ion charge of Sb would vary from + 5 for covalent bonding to − 3 for ionic bonding in the absence of electronic shielding.

We first apply the ion charge model to ^{27}AlSb. The atomic antishielding factors have been computed for different ionic states of Al by Langhoff and Hurst[13] and are given in Table II. We see in column 4 that larger effective charges than 5 are required to produce agreement between $S_{11\,\text{ionic}}$ and the experimental value of S_{11} for Al^{1+} and Al^{2+}. Al^{3+} gives approximate agreement between $S_{11\,\text{ionic}}$ and the measured S_{11} if a Sb first-neighbor charge of 5 or 6 is used. In Table III, we choose the first-neighbor charge to be 5 with the atomic antishielding factors computed for the 3+ states. We note close agreement between $S_{11\,\text{ionic}}$ and the measured S_{11} at the Al, Ga, and In nuclear positions in the seven compounds as shown in columns 6 and 7. The antishielding factors for As^{5+} and Sb^{5+} have not been computed and a comparison between $S_{11\,\text{ionic}}$ and the measured S_{11} is not possible. However, using the ion charge model with the measured S_{11} we can estimate the 5+ antishielding factors as given in Table III, column 8.

TABLE IV. Comparison of the computed $S_{11\,\text{ionic}}$ with the measured S_{11} value at Cu^{35}Cl. $S_{11\,\text{ionic}}$, S_{11}, and $\frac{16}{3}e/d^3$ are in units of 10^{15} statcoulomb cm^{-3}.

Ion	$(1-\gamma_\infty)^{a}$	$\frac{16}{3}e/d^3$	Z^*/e Cu	$S_{11\,\text{ionic}}$	$S_{11}{}^{b}$
Cl^{5+}	0.64	0.1985	1	0.13	7.9
Cl^{1-}	55	0.1985	1	10.9	7.9

[a] See Ref. 13. [b] From Table I.

The close agreement between $S_{11\,\text{ionic}}$ and the measured S_{11} at the Al, Ga, and In nuclear positions in the seven compounds supports the assumption that the ionic contribution to S_{11} is large compared to the electronic contribution and therefore also supports the Harrison-Phillips deformation model. The close agreement was achieved by using charges of + 3 at the center Al, Ga, or In atom and + 5 at the first-neighbor atoms which are the ion charges of covalent bonding. Therefore this ion charge model is successful in predicting the observed III-V compound S_{11} values when ion

TABLE III. Comparison of the computed $S_{11\,\text{ionic}}$ with the measured S_{11} values in III-V compounds. $S_{11\,\text{ionic}}$, S_{11} and $\frac{16}{3}e/d^3$ are in units of 10^{15} statcoulombs cm^{-3}.

Nuclear position	Ion state	$1-\gamma_\infty$	$\frac{16}{3}e/d^3$	Z^*/e	$S_{11\,\text{ionic}}$	$S_{11}{}^{d}$	$(1-\gamma_s)$
^{27}AlSb	Al^{3+}	3.3^{a}	0.1366	+5	2.3	2.6	...
^{69}GaP	Ga^{3+}	10.5^{b}	0.1948	+5	10.2	9.5	...
^{69}GaAl	Ga^{3+}	10.5^{b}	0.1746	+5	9.2	9.1	...
^{69}GaSb	Ga^{3+}	10.5^{b}	0.1393	+5	7.3	6.1	...
^{115}InP	In^{3+}	25.9^{c}	0.1560	+5	20.2	19.7	...
^{115}InAs	In^{3+}	25.9^{c}	0.1419	+5	18.4	16.7	...
^{115}InSb	In^{3+}	25.9^{c}	0.1161	+5	15.0	13.1	...
Ga^{75}As	As^{5+}	...	0.1746	+3	...	13.2	25
In^{75}As	As^{5+}	...	0.1419	+3	...	13.0	31
Al^{121}Sb	Sb^{5+}	...	0.1366	+3	...	13.5	33
Ga^{121}Sb	Sb^{5+}	...	0.1393	+3	...	10.7	26
In^{121}Sb	Sb^{5+}	...	0.1161	+3	...	12.3	35

[a] See Ref. 13.
[b] R. M. Sternheimer, Phys. Rev. 146, 140 (1966).
[c] R. M. Sternheimer, Phys. Rev. 159, 266 (1967).
[d] See Ref. 4.

TABLE V. Comparison of the computed $S_{11\,\text{ionic}}$ with the measured S_{11} values for I-VII compounds. $S_{11\,\text{ionic}}$, S_{11}, and $\frac{16}{3}e/d^3$ are in units of 10^{15} statcoulomb cm^{-3}.

Nuclear position	Ion state	$1-\gamma_\infty$	$\frac{16}{3}e/d^3$	Z^*/e	$S_{11\,\text{ionic}}$	S_{11}[a]
$Cu^{35}Cl$	Cl^{1-}	55[b]	0.1985	+1	10.9	7.9
$Cu^{79}Br$	Br^{1-}	101[c]	0.1711	+1	17.3	14.7
$Cu^{127}I$	I^{1-}	176[c]	0.1423	+1	25.0	22.6
$^{63}CuCl$	Cu^{+}	18[d]	0.1985	−1	3.6	6.0
$^{63}CuBr$	Cu^{+}	18[d]	0.1711	−1	3.7	4.5
^{63}CuI	Cu^{+}	18[d]	0.1423	−1	2.6	4.7

[a] From Table I.

[b] See Ref. 13.

[c] R. E. Watson and A. J. Freeman, Phys. Rev. 135, A1209 (1964).

[d] R. M. Sternheimer, Phys. Rev. 146, 140 (1966).

charges, as if there were no electronic screening, are used.

B. I-VII compounds

For I-VII compounds as CuCl, the same basic types of chemical bonding are possible: (i) covalent or homopolar with one electron from Cu and seven electrons from Cl creating the electronic bond and leaving ion cores of Cu^{1+} and Cl^{7+} and (ii) ionic or heteropolar with Cu losing its electron to Cl so that both atoms have closed electronic shells and are ions with Cu^{1+} and Cl^{1-}. The Cl ion charge would vary from + 7 for pure covalent bonding to − 1 for pure ionic bonding in the absence of electronic shielding.

We first apply the ion charge model to $Cu^{35}Cl$. The atomic antishielding factors for Cl^{5+} and Cl^{1-} have been computed by Langhoff and Hurst[13] and are given in Table IV. We note in column 5 that the antishielding factor for Cl^{5+} produces a value of $S_{11\,\text{ionic}}$ that is very much smaller than the measured S_{11}. On the other hand, the Cl^{1-} antishielding factor with a first-neighbor charge of + 1 gives approximate agreement between $S_{11\,\text{ionic}}$ and the measured S_{11}. Table V in columns 6 and 7 shows approximate agreement between $S_{11\,\text{ionic}}$ and the measured S_{11} at Cl, Br, and I nuclear positions when the charge of − 1 antishielding factors are used. At the Cu nuclear positions, the measured S_{11} are in better agreement with $S_{11\,\text{ionic}}$ computed with a first-neighbor charge of 1 than for large integer charges. This behavior is in agreement with the charge states used at the Cl, Br, and I nuclear positions.

The approximate agreement between the magnitudes of $S_{11\,\text{ionic}}$ and the measured S_{11} in Table V suggests that the computed atomic antishielding factors are good approximations of the antishielding factors in the solid. For the I-VII compounds, this simple ion charge model predicts within 30% or less the measured S_{11} values at Cl, Br, and I nuclear positions when ion charges as if there were heteropolar bonding are used.

In conclusion, the ion charge model does predict the magnitudes and variation of magnitudes of the experimental S_{11} from compound to compound in III-V and I-VII semiconductors. The resulting ion charge description of III-V compounds as approximately homopolar and I-VII compounds as approxiimately heteropolar supports the ionicity theories of Phillips[1] and Harrison.[2]

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