The selection rules on L and S cause a number of partial widths to vanish. The measurements of these widths can therefore give information about the type of coupling.

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Neutron Coherent-Scattering Amplitudes of Ga, In, As, and Sb†

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Neutron-diffraction data obtained from the compounds GaAs, GaSb, InAs, and InSb lead to the following neutron coherent-scattering amplitudes: $f_{Ga} = (0.72 \pm 0.01) \times 10^{-12}$ cm, $f_{In} = (0.39 \pm 0.01) \times 10^{-12}$ cm, $f_{As} = (0.64 \pm 0.01) \times 10^{-12}$ cm, and $f_{Sb} = (0.54 \pm 0.01) \times 10^{-12}$ cm. The data were also used to evaluate the Debye characteristic temperature for the compounds in use; the resulting Debye temperatures are 175°K for InSb, 240°K for InAs, 235°K for GaSb, and 247°K for GaAs. The neutron wavelength employed was 1.391 Å.

I. INTRODUCTION

INFORMATION on neutron coherent-scattering amplitudes is still lacking for a few of the naturally occurring elements. The present experiment was instigated to determine the scattering amplitudes primarily of Ga and In. During the course of the experiment, it was discovered that In had been measured previously[1]; however, it is believed that the accuracy of the present result is an improvement over the earlier measurement. As a consequence of the particular compounds used in the measurements for Ga and In, values for the scattering lengths of Sb and As could also be determined. Measurements on the latter elements have been previously reported[2] but, again, the accuracy is somewhat better in the present experiment.

The intermetallic compounds, GaAs, GaSb, InAs, and InSb, were employed in the present measurements on account of their common cubic structure and their availability in semiconductor purity. The customary usage of the metal sesquioxides in this type of measurement was not employed in this instance on account of their more complex structure and unresolved diffraction patterns. Since the Sb and As scattering amplitudes are not known as accurately as that of O, two compounds of each element were used in order to improve the accuracy of the Ga and In measurements.

[1] S. S. Sidhu, L. Heaton, and M. H. Mueller, J. Appl. Phys. 30, 1323 (1959).
[2] C. G. Shull and E. O. Wollan, Phys. Rev. 81, 527 (1951).

II. EXPERIMENTAL

The measurements were made on one of the neutron diffractometers at the Omega West Reactor. The neutron beam reflected from the (111) planes of a Pb monochromating crystal had a cross-sectional area of $1\frac{1}{2} \times 1\frac{1}{2}$ in., an intensity of 10^6 neutrons/cm²-sec at the sample position, and a wavelength of 1.391 Å. The compounds were contained in a 3-in.-diam disk-type holder made of Ti-Zr alloy. The total wall thickness of the holder was 0.050 in. and the neutron transmission of the empty holder was 95%.

Pertinent physical data entering into subsequent calculations are given in Table I for each compound. The measured neutron transmissions given in Table I were obtained by placing the sample in the diffracted neutron beam from the (111) planes of a pressed nickel-powder sample; these measured values were used to determine the absorption correction for the samples. The calcu-

TABLE I. Physical data on samples used in the present experiment.

Compound	Theoretical density (gm/cm³)	Sample thickness (gm/cm²)	Measured transmission[a]	Calculated transmission[a]	Lattice constant (Å)
GaAs	5.37	1.03	0.87	0.88	5.636
GaSb	5.62	0.79	0.90	0.91	6.096
InAs	5.67	0.94	0.56	0.58	6.058
InSb	5.78	0.91	0.64	0.65	6.476

[a] These values include the Ti-Zr sample holder.

lated transmissions, obtained by using the total neutron scattering cross sections of the elements at 0.0425 eV, are also listed for comparison purposes. It is not understood why the calculated transmissions are slightly higher than the measured values.

Diffraction data for each compound were taken over a scattering angle range from 10° to 85° at maximum intervals of 0.2°; over the lower angle scattering region, peaks were scanned at 0.1° intervals. In all compounds, the diffraction peaks were well resolved and peak locations agreed within 0.1° with the calculated values using the lattice constants given in Table I. In general, the statistical accuracy of the diffraction peak areas was estimated to be 2% or better over the low-angle scattering range from 20° to 40°; over the high-angle range from 40° to 85°, the statistical accuracy was 5% or better. An exception to the above was the (200) reflection which was always of small intensity; the accuracy of this peak was usually determined to no better than 5%. The diffractometer was calibrated on an absolute basis by using a pressed Ni-powder sample as a standard; the scattering amplitude of Ni was taken as 1.03×10^{-12} cm. The Ni sample was alternated with the four compounds and the resulting constant obtained for the absolute calibration of the spectrometer was estimated to have an accuracy of about 2%.

All of the compounds in Table I possess the zincblende structure (face-centered cubic). Using InSb as an example, the following structure equations result for the above crystal type at a scattering angle of 0°:

$$F_{hkl}^2 = 16(f_{In}^2 + f_{Sb}^2) \text{ when } h+k+l \text{ is odd}, \tag{1}$$

$$F_{hkl}^2 = 16(f_{In} + f_{Sb})^2 \text{ when } h+k+l$$
$$\text{is an even multiple of } 2, \tag{2}$$

$$F_{hkl}^2 = 16(f_{In} - f_{Sb})^2 \text{ when } h+k+l$$
$$\text{is an odd multiple of } 2. \tag{3}$$

The values of the structure factor F_{hkl}, as calculated from the various diffraction peak data, are shown graphically for the four compounds in Figs. 1–4. Details concerning the procedures of this calculation have been discussed in earlier publications.[1,2] The customary plot

of $\log F_{hkl}^2$ versus $(\sin\theta/\lambda)^2$ is shown which should result in straight lines for each set of hkl planes associated with the above three equations. For the present angular scattering range, the (200) plane is the only reflection associated with Eq. (3). The error limits shown on the points represent the combined statistical and instrumental errors. The chief instrumental error arose from the determination of the spectrometer constant using the Ni standard.

It should be noted that the (200) diffraction peak was useful in evaluating the scattering amplitudes in spite of its small intensity and relatively large percentage error. Since the intensity of this reflection is proportional to the square of the difference of the scattering amplitudes of the elements, it is a sensitive indicator of their relative magnitudes. In the case of GaAs, no (200) peak was observed; however, in order to use this fact in the calculations, it was assigned a value equal to one-half the minimum detectable scattering intensity (see Fig. 1). The fact that no peak appeared at the (200) position when the scattering amplitudes of the two elements were approximately equal was also construed as evidence that second-order reflections from the (400) planes were negligible. Since the (400) diffraction peak was especially large in the case of GaAs, it was concluded that second-order contributions to the (200) peak in the other three compounds were also insignificant.

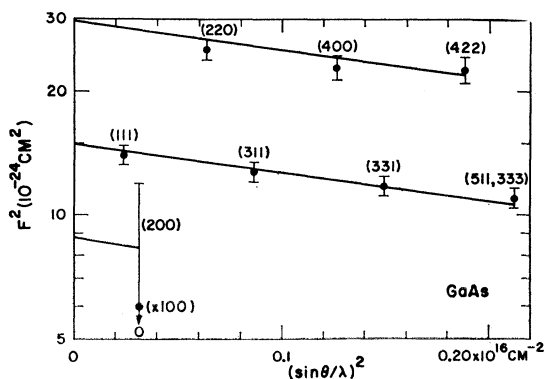FIG. 2. Square-of-structure factor for GaSb versus $(\sin\theta/\lambda)^2$.

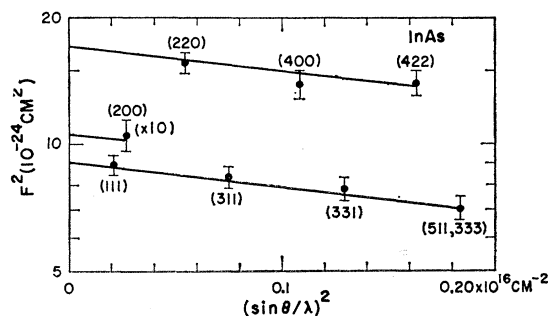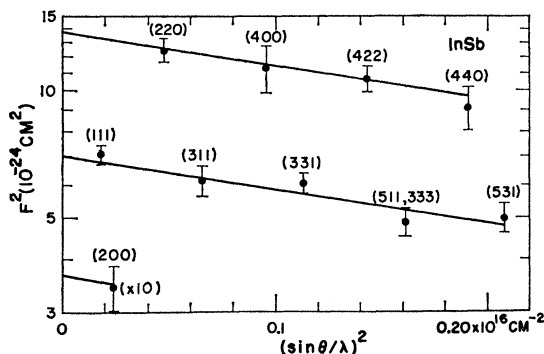FIG. 1. Square-of-structure factor for GaAs versus $(\sin\theta/\lambda)^2$.

FIG. 3. Square-of-structure factor for InAs versus $(\sin\theta/\lambda)^2$.

FIG. 4. Square-of-structure factor for InSb versus $(\sin\theta/\lambda)^2$.

III. RESULTS

The straight lines shown in Figs. 1–4 were obtained by a least-squares analysis applied to the data points of all four compounds. This resulted in 34 equations to determine the 4 scattering amplitudes. Each point was assigned a statistical weight proportional to the inverse square of the indicated errors on the graphs.[3] Equal slopes were assumed for the lines associated with the three sets of hkl planes in each compound. The intercepts of the straight lines with the y axis, which give the structure factors at $(\sin\theta)/\lambda=0$, were used to calculate the scattering amplitudes from the four compounds using Eqs. (1), (2), and (3). The neutron coherent scattering amplitudes obtained from the above

TABLE II. Neutron coherent-scattering amplitudes (in cm) for Ga, In, As, and Sb.

Element	Scattering amplitude from present experiment	Scattering amplitude from earlier experiments (Refs. 1 and 2)
Ga	$(0.72\pm0.01)\times10^{-12}$	...
In	$(0.39\pm0.01)\times10^{-12}$	$(0.36\pm0.02)\times10^{-12}$
As	$(0.64\pm0.01)\times10^{-12}$	$(0.63\pm0.02)\times10^{-12}$
Sb	$(0.54\pm0.01)\times10^{-12}$	$(0.54\pm0.02)\times10^{-12}$

[3] Treating these combined errors as statistical appears justifiable since the spectrometer constant derived from the Ni standard varied among the four compounds. A separate least-squares analysis, carried out using only counting errors associated with the data points, gave essentially the same final results for the scattering amplitudes.

TABLE III. Debye temperatures for the compounds InSb, InAs, GaSb, and GaAs.

Compound	Observed $W/\sin^2\theta$	Calculated Debye temperature[a] (°K)	Previous Debye temperature values (Ref. 3) (°K)
InSb	0.48	175	...
InAs	0.32	240	...
GaSb	0.34	235	233
GaAs	0.40	247	314

[a] Assuming nuclear mass equal to one-half molecular weight.

analysis are given below in Table II together with previous literature values. All of these elements possess positive scattering amplitudes.

Considering the experimental error limits, both the present and previous measurements are compatible for the elements which can be compared. The As and Sb results agree especially well with previous values. The fact that the least-squares analysis results in lines which lie within the error limits on all the data points substantiates the consistency of the data among the four compounds.

The Debye temperatures characteristic of the four compounds used in the experiment can be evaluated from the slopes of the straight lines in Figs. 1–4. Table III gives the experimental value of $W/\sin^2\theta$ where W is the Debye-Waller temperature factor. In calculating the Debye temperature from the above quantity, the nuclear mass has been taken as one-half that of the molecular weight of the compound. The present Debye temperature values compare favorably with an earlier value in the case of GaSb but differ appreciably for GaAs.[4] The present values seem consistent in that they increase monotonically with increasing melting points.

[4] *International Tables for X-ray Crystallography* (The Kynoch Press, Birmingham, England, 1962), Vol. 3, p. 241.