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# IX-4. Shubnikov-de Haas Effect and Electron Band Structure of Cadmium Arsenide

I. ROSENMAN

*Laboratoire Central des Industries, Electriques*
*33, Avenue du Général Leclerc*
*92-Fontenay-Aux-Roses, France*

Shubnikov de Haas effect has been observed in oriented *n*-type $Cd_3As_2$ single crystals, in the concentration range $2\text{-}3\times10^{18}cm^{-3}$. Both temperature and orientation dependence of the effect, have been studied.

A $1/B$ linear in time, programming for the magnetic field $B$, was used permitting the use of electronic filtering.

Curves were fitted by least squares method with the aid of a UNIVAC 1107 electronic computer.

Main results are: a single revolution ellipsoid about $c$ 4-fold axis with $m_{//}/m_0=0.050\pm0.001$ and an anisotropy factor $X=1.18$.

Dingle temperature is $16.8\pm1°K$.

## § 1. Introduction

Cadmium Arsenide ($Cd_3As_2$) is a *n*-type high mobility degenerate semiconductor, with a tetragonal crystallographic system.[1]

Using the high mobility and degeneracy properties it is possible to obtain information on the band structure by studying the de Haas van Alphen type oscillations of the magnetoresistance, arising from the quantization of the electron orbits in a high magnetic field. Theory of the so called Shubnikov-de Haas effect (SdH) has been done by Adams and Holstein.[2]

Some of the results obtained by the studying of the Shubnikov-de Haas effect in $Cd_3As_2$ have been shortly reported elsewhere.[3]

## § 2. Experimental Methods

The magnetic field $B$, of a 50 kG Westinghouse Superconducting coil was programmed in such a manner that $1/B$ varied linearly with time, thus obtaining a periodic in time, variation of the resistivity (periods about 10 seconds). This fact has permitted to make use of a very low frequency electronic filter to cancel out the monotonic variation of the resistivity and enabled us to measure very small relative amplitudes of the resistivity oscillations. Actually the oscillatory voltages amplitudes were in the range of $2\times10^{-2}\mu V$ to $2\mu V$, corresponding to relative resistivity variations of $5\times10^{-2}$ to $5\times10^{-4}$. Voltages were plotted on a *X-Y* recorder, $X$ side receiving an *e.m.f.* proportional to $1/B$.

SdH effect has been observed in a range of temperatures extending from 1.5°K to 50°K. The temperatures, measured with a 33 ohms, 1/10 watt Allen Bradley resistor, were regulated to 0.2°K.

The samples were x-Ray oriented monocrystals grown from the vapor phase.[4]

Samples with $c$ 4-fold axis in the length as well as in the width were used.

Electron concentrations in the samples were in the range $(2\sim2.6)\times10^{18}$ cm$^{-3}$, while mobilities at 4.2°K varied from 50,000 to 80,000 cm$^2$/V sec, according to the sample. Both rotation schemes were used in the experiments, the "transversal" about the current axis and the "transversal-to-longitudinal", with respect to the magnetic field. Table I gives the characteristics of the samples.

Table I. Samples Characteristics.

| Sample | Orientation (1=length) | Concentration $n$(cm$^{-3}$) | Mobility (cm$^2$/V sec) | |
|---|---|---|---|---|
| | | | 300°K | 4.2°K |
| MP 1 | $C//1$ | $2.75\times10^{18}$ | 9100 | 51.300 |
| MP 3 | $C\perp1$ | $2.13\times10^{18}$ | 14500 | 76.200 |
| MP 4 | $C\perp1$ | $2.60\times10^{18}$ | 14000 | 69.300 |

## § 3. Results and Interpretation

Figure 1 represents the oscillatory part of the magnetoresistance for two temperatures and two orientations

$$(c//B \text{ and } c\perp B)\ .$$

### 3.1. *Fermi surface structure*

No matter what the orientation of the sample was, we have observed only a single period of

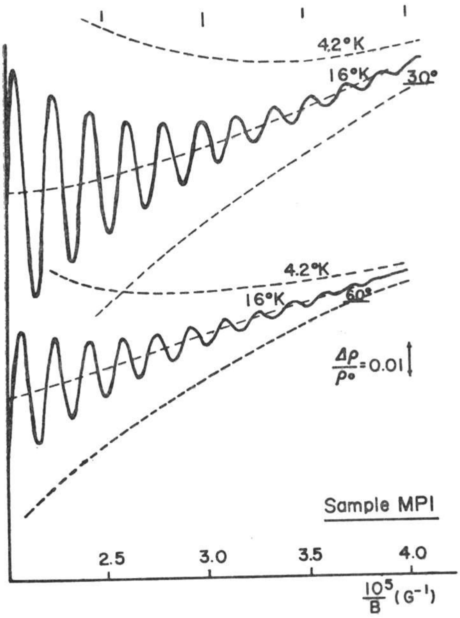


Fig. 1. Oscillations in the magnetoresistance, for two orientations of the crystallographic axes, with respect to the magnetic field $B$.

oscillation, it proves that in the range of concentrations used there is only one type of carriers (electrons) which participate to SdH effect (see Fig. 2), and that if one has a multivalley structure, the constant energy surfaces are oriented in such a manner that for each orientation there is only one extremal cross-section of the F.S.

The period $P$ (in reciprocal magnetic field) of the oscillation is related to the extremal cross-section $S_m$ of the Fermi Surface, in $k$ space, by the Lifschitz-Onsager relation,

$$P=\frac{2\pi e}{\hbar}\frac{1}{S_m}\,. \tag{1}$$

Then supposing a Fermi surface consisting of ellipsoids, they must have their axis oriented in the same direction, and one gets the following equation for the angular variation of the period $P$.

$$P^2(\theta)=A\sin^2\theta+B\cos^2\theta\ , \tag{2}$$

$\theta$ being the angle between the major axis (if $A<B$) and the magnetic field.

We have made a least square fit for the angular variation of the period; $P^2$ versus $\cos^2\theta$ must then be a straight line.

A comparison of the experimental values and the least squares fit, is shown in Fig. 2, for three different samples. It can be seen that the fit is good, and all three samples give, to 1%,

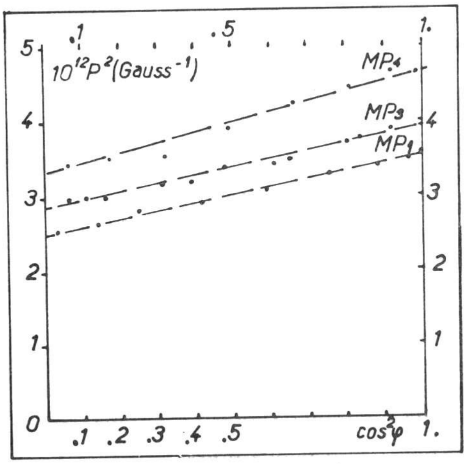


Fig. 2. Period angular variation, least square fit, $P^2$ is the square of the period. $\varphi$ is the angle between the $c$ 4-fold axis and the magnetic field.

the same anisotropy ratio

$$X=(B/A)^{1/2}=1.18\pm0.01\ ,$$

and

$$\theta=\varphi\ ,$$

$\varphi$ being the angle between the $c$ 4-fold axis and the magnetic field $B$.

We can conclude that the $c$ 4-fold axis of the crystal is the major axis of the ellipsoids. Now we find the number of ellipsoids by comparing the electron concentration in the F.S., obtained from Hall effect measurement with that obtained from the SdH periods, the latter gives the following value for the concentration $n$ of the carriers:

$$n=\frac{N_v}{3\pi^2}\left(\frac{2e}{\hbar}\right)^{3/2}\left(\frac{1}{P_1P_2P_3}\right)^{1/2}. \tag{3}$$

$N_v$ is the number of ellipsoids, $P_i$ the periods observed in the 3 principal directions.

For sample MP 1, one has

$$P_1=1.89\times10^{-6}G^{-1}\qquad P_2=P_3=1.60\times10^{-6}G^{-1}.$$

That is

$$n_{\mathrm{SdH}}=2.59\times10^{18}N_v(\mathrm{cm}^{-3})\ . \tag{4}$$

From Hall effect one gets

$$n_H=2.74\times10^{18}(\mathrm{cm}^{-3})\ . \tag{5}$$

Comparing eqs. (4) and (5) gives

$$N_v=1\ .$$

For sample MP 3

$$P_1=2.01\times10^{-6}G^{-1}\qquad P_2=P_3=1.72\times10^{-6}G^{-1}$$

$$n_{\mathrm{SdH}}=2.31\times10^{18}N_v(\mathrm{cm}^{-3})\ , \tag{4'}$$

and

$$n_H = 2.13 \times 10^{18} (\mathrm{cm}^{-3}) \,. \qquad (5')$$

Comparison gives:

$$N_v = 1 \,.$$

Thus we can conclude that there is only one ellipsoid, which is a revolution ellipsoid about 4-fold *c* axis, the ellipsoid is elongated in the *c* direction ($P_2 < P_1$).

### 3.2. *Effective mass tensor and Dingle temperature*

By combining the magnetic field variation and the temperature variation of the SdH effect, we have determined both the effective masses and the Dingle temperature.

The variation of the oscillatory part of the magnetoresistance is given by the following relation[2]:

$$\frac{\Delta\rho}{\rho_0} = -\frac{\Delta\sigma}{\sigma_0} \sim B^{-1/2} T \frac{e^{-(2\pi^2 k m^* T_D/\hbar e B)}}{\sinh(2\pi^2 k m^* T/\hbar e B)} \times \cos\left(\frac{2\pi}{PB} - \frac{\pi}{4}\right),$$

—$\rho_0$, ($\sigma_0$) is the resistivity (conductivity) without magnetic field $B$.
—$T_D$ is the Dingle temperature.
—$m^*$ is the cyclotron mass.
—$P$ is the oscillation period.
This formula is valid only when $|\Delta\rho/\rho_0| \ll 1$, which is our case.

Owing to the fact that the argument in the hyperbolic sine is in the range 0.5–2, we cannot approximate the sinh by the exponential.

For this reason we have programmed a UNIVAC 1107 electronic computer to make a non linear least squares fit of the experimental data to the Adams-Holstein formula.[6]

This was done in the following manner: for each temperature, the fit of the magnetic field dependence was made for fixed Dingle temperature allowing the mass $m^*$ to vary, thus obtaining a set of pairs ($m^*$, $T_D$) for each temperature. Doing this for several temperatures we have chosen finally the values of $m^*$ and $T_D$ which fit simultaneously the experimental curves for different temperatures. We have followed the method described by Soule, McClure and Smith.[6] Figure 3 gives an example of the UNIVAC 1107 fit of the experimental curves for several temperatures, with *c* axis parallel to the magnetic field.

The cyclotron mass found for the *c* axis parallel to the magnetic field $B$, is

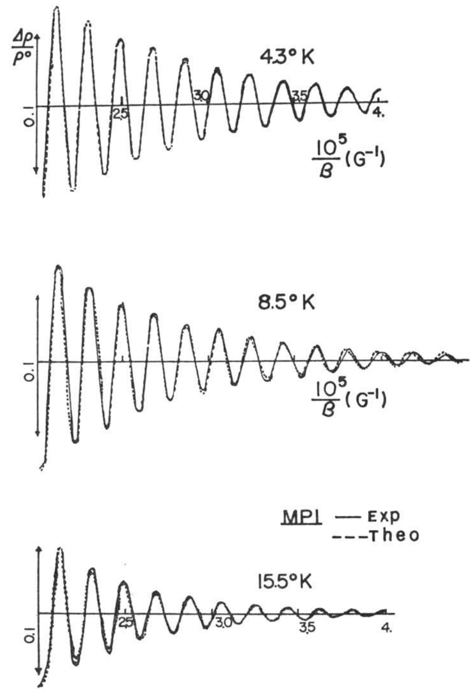


Fig. 3. Least square fit for the experimental curves.

$$\frac{m_{/\!/}}{m_0} = 0.050 + 0.001 \,.$$

The Dingle temperature is, for the same orientation

$$T_D = 16.8 \pm 1\,^\circ\mathrm{K} \quad \text{for} \quad \mathrm{MP}\ 1 \,.$$

This Dingle temperature is higher than that expected from the mobility calculation, which is:

$$T_\mu = \frac{\hbar}{\pi k \tau} = \frac{e\hbar}{\pi k m \mu} = 1.76\,^\circ\mathrm{K} \quad \text{for} \quad \mathrm{MP}\ 1 \,.$$

This discrepancy may have its origin in the different kinds of defects of the crystal such as inhomogeneities, etc....

The determination of the cyclotron mass in the other directions, although less precise, gives results in fair agreement with the angular variation of the period:

$$\frac{m_\perp^*}{m_0} = 0.060 \pm 0.005 \quad \text{for} \quad \theta = 90^\circ \,.$$

From this one gets an anisotropy factor

$$X = \frac{m_\perp^*}{m_{/\!/}^*} = \frac{0.060}{0.050} = 1.20$$

which agrees with the 1.18 found from period variation.

We have also observed very small oscillation in the Hall coefficient, of the order of $10^{-3}-10^{-4}$.

## § 4. Conclusion

The $n$-type $Cd_3As_2$ Fermi-Surface has been determined, in the concentration range where only one type of carriers is present. It is found to be a single ellipsoid elongated in the $c$ direction with an effective mass in this direction $m=0.050\,m_0$ and an anisotropy factor $X=1.18$.

Experiments are made now on heavy doped ($n\sim10^{19}\text{cm}^{-3}$) single crystal to determine if there is a second type of carriers as it has been suggested from classical transport effects.[1]

**Acknowledgement**

We are indebted to Professor J. Tavernier for his interest and helpful discussions during this work.

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## DISCUSSION

**Moss, T. S.:** Have you tried to measure specimens with much lower carrier concentration, as your reported specimens would have considerable band filling?

**Rosenman, I.:** As yet we have not tried to measure SdH effect on sample with much lower carrier concentration, because we did not success to change the concentration in a wide range. Concentration observed varied from $1.7\times10^{18}\text{ cm}^{-3}$ to $2.6\times10^{18}\text{ cm}^{-3}$. Recently we have succeeded in doping our samples up to $5\times10^{18}\text{ cm}^{-3}$ and we are measuring SdH effect on these samples to see both non-parabolic effects and the existence of a second band. The main difficulty in doping is the existence of a solid phase transformation at 578°C; this implies that doping must be done in vapor phase, as we have in fact done.

**Stratton, R.:** Is the Adams-Holstein formula quoted by you valid if the argument of the sin factor is less than one? I would expect that you should then use more terms of the full series.

**Rosenman, I.:** In our computer calculation we have taken into account not only the first term in Adams-Holstein formula, but also the first harmonic, which was sufficient.