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Measurement of Cyclotron Masses in Re03

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MEASUREMENT OF CYCLOTRON MASSES IN ReO_3

by

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SCOPE AND CONTENTS:

The cyclotron masses in ReO_3 have been determined from the temperature dependence of the dHvA amplitude. Three frequency branches α, β, γ_1 in the (110) plane were investigated. The dHvA effect was detected by the low-frequency field modulation technique, using field values of 35-55 kOe at temperatures below 2.172 K. The cyclotron masses for α, β, γ γ branches varied between (0.56-0.72) m_o, (0.75-0.96) m_o, and (0.6-1.0) m_o, respectively.

Measured effective mass values for the extremal orbits of the three branches are in reasonable agreement with the theoretical prediction of Matthiess (1969) calculated by the augmented plane wave (APW) method. A frequency of 73.4 MG near the [110] direction with an effective mass of 1.07 m_o was detected in addition to the six frequency branches which were previously reported. This is in agreement with Matthiess' prediction.

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CHAPTER I

INTRODUCTION

The compound ReO_3 is a red transition-metal oxide, which exhibits metallic electrical conductivity. In addition to its importance as a transition metal oxide, ReO_3 is interesting because of its relatively simple crystal structure. This structure is closely related to certain classes of materials such as the perovskites (ABO_3) and the tungsten bronze (A_xWO_3) where A is an alkali metal, copper or silver.

Single crystals of ReO_3 were first prepared by Ferretti et al (1965). They found that the electrical conductivity at 77 K was 2.5×10^6 $(\Omega\ cm)^{-1}$. This is the same order of magnitude as the conductivity of copper. Further work was done in ReO_3 using nuclear magnetic resonance by Narath and Barham (1968) who found that the conduction electron states of ReO_3 at the Fermi level are derived mainly from atomic d states. They also found that the conduction band of the metals ReO_3 and Na_xWO_3 are very similar.

The first de Haas-van Alphen (dHvA) measurements on ReO_3 were reported by Marcus (1968). He measured three dHvA frequency branches and the cyclotron mass of one branch for three different magnetic field directions near the [111] direction. Mattheiss (1969) carried out a band structure

calculation for ReO_3 based on the augmented-plane wave (APW) method and determined the Fermi surface of ReO_3. He calculated the three dHvA frequency branches observed by Marcus and predicted three additional frequency branches. He also calculated the cyclotron mass for closed orbits on the ReO_3 Fermi surface. Phillips and Shanks (1971) reported the three other frequency branches predicted by Mattheiss and the cyclotron mass for one magnetic field direction. Schirber et al (1972) determined hydrostatic pressure derivatives of dHvA frequencies at the symmetry directions. They reported significant deviations from the prediction of free electron scaling.

Mattheiss shifted his bands relative to each other by several volts in order to fit his energy band calculations to the optical data of Feinleib et al (1968). He also used one adjustment parameter to gain agreement between the calculated masses and the mass measurement by Marcus. The previous dHvA effective mass measurements of Marcus were limited only to one frequency branch for field directions near the [111] direction. The purpose of this work is to present detailed cyclotron mass measurements for the three electron like sheets of the Fermi surface for magnetic field directions in the (110) plane. A detailed cyclotron mass measurement is of importance because once the cyclotron mass has been determined the Dingle temperature and the g-factor

can be deduced. It is also of interest to compare the observed masses with the theoretical values that have been calculated.

CHAPTER II

THEORY

A. de Haas-van Alphen Theory

The de Haas-van Alphen (dHvA) effect is an oscillatory variation of the magnetic susceptibility, which is periodic in the reciprocal of the field strength.

Onsager, from a semiclassical argument, showed that the periodicity of the dHvA oscillations is simply related to a maximum cross sectional area of the Fermi surface in a plane normal to the magnetic field.

The detailed expression for the oscillatory magnetization was given by Lifshitz and Kosevich (L.F.) in 1955. Their expression for the oscillatory magnetization (in polar coordinate) is:

$$M = D(H)\left[H - \frac{1}{F}\frac{\delta F}{\delta \theta}\hat{\theta} - \frac{1}{F\sin\theta}\frac{\delta F}{\delta \phi}\hat{\phi}\right] \times$$

$$\sum_{r=1}^{\infty}\left[I_r K_r / r^{3/2}\right] \sin\left[2\pi r\,(F/H - \gamma) \pm \frac{\pi}{4}\right]$$

$$\cos\left(\frac{\pi}{2}\, r\, g\, \frac{m^*}{m}\right) \qquad \text{(II-1)}$$

where

$$D(H) = -\frac{ehA}{4\pi^4 m^*}\left(\frac{2\pi eH}{h}\right)^{1/2}\left|\frac{\delta^2 A}{\delta K_H^2}\right|^{-1/2}$$

In this expression A is an extremal cross sectional area of the Fermi surface, $\frac{\delta^2 A}{\delta k_H{}^2}$ is the curvature factor of the Fermi surface at the extremum, F is the dHvA frequency which is related to an extremal cross section of the Fermi surface A by the relation $F = \frac{\hbar}{2\pi e} A$ (II-2)

The (+) and (-) signs in the sin terms are used for the maximum and minimum cross sectional areas, respectively. The cyclotron mass m* is described by

$$m^* = \frac{\hbar^2}{2\pi} \left(\frac{\delta A}{\delta E} \right)_{k_H} \qquad \text{(II-3)}$$

where E is the electron energy at the Fermi surface. I_r represents the temperature dependence of the dHvA effect and is given by

$$I_r = \frac{X_r}{\sinh X_r} \qquad \text{(II-3)}$$

where

$$X_r = 2\pi^2 r \frac{k_B T m^*}{e \hbar H} = 14.69 \; r \; m^* \; T/H \qquad \text{(II-4)}$$

(k_B is the Boltzmann factor).

The broadening of the Landau levels in equation (1) is described by

$$k_r = e^{-2\pi r (\Gamma/\hbar\omega_c)} = e^{-2\pi^2 r (m^* k_B T_D / eH\hbar)} = e^{-14.69 \frac{m^* T_D}{H}} \qquad \text{(II-5)}$$

where the Dingle temperature T_D is related to the half-width (Γ) of the Lorentzian curve describing the broadening of the Landau levels by

$$T_D = \Gamma / \pi k_B \qquad \text{(II-6)}$$

Finally the factor $\cos\left(\frac{r\pi}{2}\, g\, m^*/m\right)$ is the correction factor for the spin, and g is a splitting factor which is equal to 2.0023 for free electron.

The cyclotron mass m^* can be determined from the temperature dependence of the dHvA amplitude. From eq. (II-4) the temperature dependence of the amplitude is described by

$$\mathrm{Amp} = C\,\frac{X_r}{\sinh X_r} \qquad \text{(II-7)}$$

where c is some factor which does not depend on temperature. By expanding the sinh function, the amplitude may be written as

$$\mathrm{Amp} = C\,\frac{2X_r}{e^{X_r} - e^{-X_r}} = 2\,C\,X_r\,e^{-X_r}\,(1-e^{-2X_r})^{-1} \qquad \text{(II-8)}$$

It is clear that the higher harmonics of the oscillation are damped. X_r is equal to 3r for free electrons in a field of 50 KG and at a temperature of 1 K. The damping factor $e^{-2X_r} = e^{-2\times 3} \ll 1$ for the fundamental frequency. Therefore, we are able to neglect the factor e^{-2X_r} for high cyclotron masses. By the above argument eq. (II-8) can be written as

$$\mathrm{Amp} = c\,2X_r\,e^{-X_r}$$

or

$$\ln \mathrm{Amp} = \ln\,(2c\,X_r e^{-X_r})$$

Therefore

$$\ln(\mathrm{Amp}/T) = 14.69\ m^*T/H + c \qquad \text{(II-9)}.$$

Thus, the cyclotron mass can be determined by finding the slope of the plot of ln (Amp/T) vs. temperature.

It is possible to determine the Dingle temperature from the variation of amplitude with field when the cyclotron mass m* is known from the temperature variation of amplitude. In the presence of a finite temperature the Landau levels are not perfectly sharp but are broadened. This effect arises ~~from~~ the finite lifetime of electron states caused by collisions, the lifting of magnetic degeneracy of the electron orbits by the lattice potential and the effects of the dislocation in the crystal. From eq. (II-1) the Dingle temperature is determined from the slope $14.69\ m^*T_D$ of a plot of

$$\ln\left[\frac{\mathrm{Amp}}{T}\sqrt{H}\ \sinh\ \frac{14.69m^*\ T}{H})\right]\ \text{vs.}\ \frac{1}{H}\ .$$

B. Band Structure and Fermi Surface of ReO_3

ReO_3 is body centered cubic crystal with the lattice parameter 3.743 Å. The density of the material is 6.91 gms/cm^3.

Mattheiss calculated the band structure for ReO_3 in three stages. He used an APW calculation at symmetry points in the Brillouin zone in the first stage. Next, he used the method of Slater-Koster's LCAO (linear-combination of atomic

orbitals) to fit the APW results at symmetry direction to the energy bands throughout the Brillouin zone. The fitting procedure that he used included states arising from the rhenium 5d and oxygen 2p bands. He also took account of the effects of spin-orbit coupling among the rhenium 5d states. Finally, he adjusted the LCAO or tight-binding parameters which affect the energy separation between oxygen 2p and rhenium 5d energy bands to fit the experimental optical data of Feinleib et al (1968) and cyclotron masses measured by Marcus (1968).

Mattheiss found several Fermi surface sheets, which he labelled α, β, γ. Each sheet corresponds to an electron-like surface centered about Γ. The α and β sheets are closed, while the γ sheet is open along $\langle 110 \rangle$ directions. The α, β and γ Fermi surface sheets contains .093, .171 and .736 electrons per rhenium atom. A three-dimensional sketch of the Fermi surface sheets is shown in Fig. 1. The α sheet is rather circular in the (100) plane and slightly squared off in the (110) plane. The reverse is true for the β sheet. The γ sheet has two closed extremal orbits when the magnetic field is along the [100] direction. One is electron-like γ_1, and the other is hole-like γ_2. Another extremal orbit γ_3 which is electron-like exists on the γ sheet when the magnetic field is near the [111] direction. There is also γ_4, a hole-like orbit which is analogous to γ_3. It can be visualized on a hole surface similar to the γ surface but enclosing all

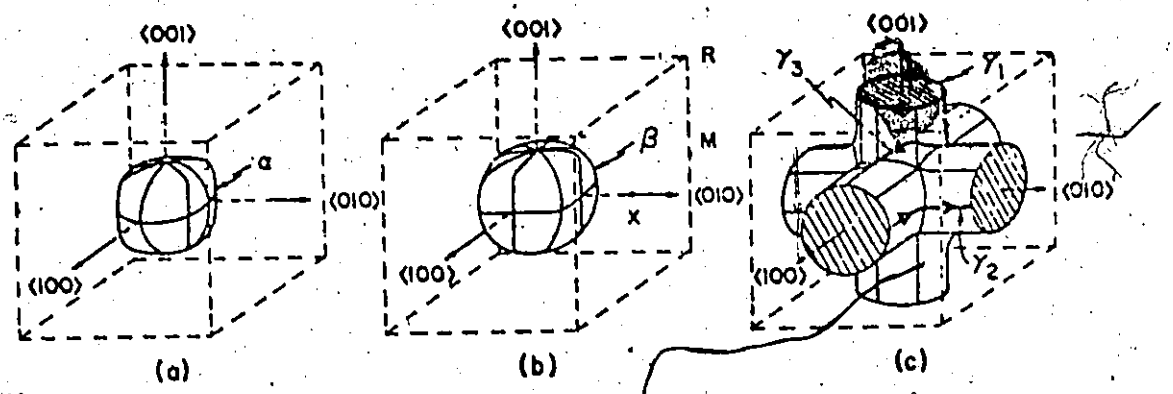

FIG. 4. Three-dimensional sketches of the three electron sheets of the APW FS in ReO_3 (after Mattheiss; Philips and Shanks added the γ_3 orbit to this figure).

Figure 1

space not inside the γ surface.

In addition to these orbits, Mattheiss predicted an orbit which involves magnetic breakdown from the β to the γ Fermi surface sheets when the magnetic field is along the [110] direction. The extremal area and cyclotron mass of this orbit are $0.750 A^{\circ -2}$ (corresponding to a frequency of 78.75 MG) and $0.86\ m_o$, respectively.

Mattheiss used the Muller (1966) inversion scheme to determine the cyclotron masses for orbits for the central extremal area of the Fermi surface. The results for the α, β and γ_1 orbits for (100) and (110) planes, are shown in Fig. 2. It should be mentioned that these results are the adjusted cyclotron masses.

APW cyclotron masses for closed orbits on ReO_3 Fermi surface.

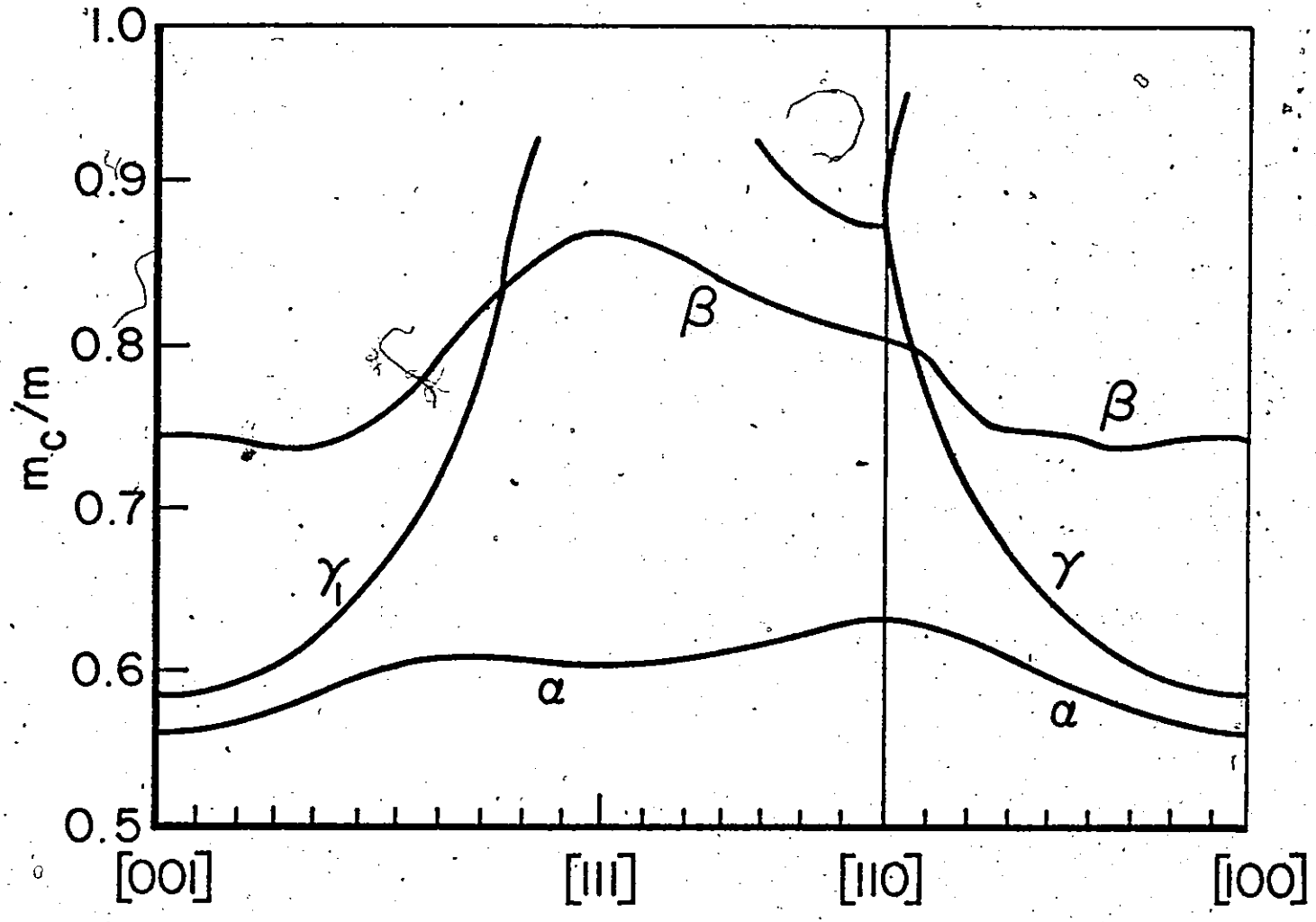
1.0
0.9
0.8
0.7
0.6
0.5
m_c/m
[001]
[111]
[110]
[100]
β
γ_1
α
β
γ
α

Figure 2

CHAPTER III

EXPERIMENTAL TECHNIQUE

The low frequency-modulation technique was used to detect dHvA oscillations. In this technique a small magnetic field h_0, parallel to H_0, is produced by passing a current through a modulation coil. The time derivative of the magnetization M is detected by a pick-up coil at a harmonic of the modulation frequency. The magnetic field at any time can be written as $H + h_0 \sin \omega t$. Upon substituting this field into eq. (II-1) and using the fact that $h \ll H_0$ and $\frac{2\pi F n^2}{H_0 3} = \frac{\alpha h}{H} \ll 1$ the magnetization can be written in the form

$$M = A(H_0) \left[\sin (2\pi F_r/H_0) \cos (\alpha \sin (\omega t)) - \cos (2\pi F_r/H_0) x \sin (\alpha \sin \omega t) \right] \qquad \text{(III-1)}$$

where $\alpha = 2\pi Fh/H_0$.

Equation (III-1) can be expanded into its harmonic components of ω by using the property.

$$\cos (x \sin \theta) = J_0(x) + 2 \sum_{N=1}^{\infty} J_{2N}(x) \cos (2N\theta)$$

and $\sin (x \sin \theta) = 2 \sum_{N=1}^{\infty} J_{2N+1}(x) \sin ((2N+1)\theta)$

Then the time derivative of (III-1) can be written as

$$\frac{\delta H}{\delta t} = -A(H_0) \sum_{n=1}^{\infty} [2n\omega J_n(\alpha) \sin(n\omega t + \frac{n\pi}{2}) \times \sin(\frac{2\pi F_r}{H_0} + \phi + \frac{n\pi}{2})] \quad \text{(III-2)}$$

As the field H_0 changes with time, each dHvA frequency term F_r generates a series of harmonics of modulation frequency ω.

The crystal used in the measurement was obtained from Ferretti and was approximately a cube in shape with a side dimension of 2mm. The speciman was oriented by the back reflection Laue method. It was mounted in a sample holder with an error in the crystal alignment of about half degree.

The modulation frequency was 517 Hz which was low enough to allow complete penetration of the modulation field into the sample. If this is not the case, then the Bessel function in expression (III-2) will not have the same value in all parts of the sample (Gold 1968).

The dHvA frequencies were detected at the second harmonic of 517. The detailed electronic processing has been described by Dunsworth (1972).

A 55 kG Westinghouse superconductivity solenoid was used to provide the d.c. field. The field values of 35-55 kG were used to observe the dHvA oscillations in ReO_3. Data were collected on magnetic tape and Fourier analyzed by computer. The amplitude for each frequency was found from the Fourier transform amplitude.

Great care was taken to ensure that the amplifier-detection system was highly linear and the gain of neither the oscillator power amplifier or amplifier detection system change with time.

Temperature determinations were made by measuring the liquid helium vapour pressure with a Texas Instrument precision pressure gauge. All data were taken below the λ point (2.172 k) to ensure that the liquid and vapour were in equilibrium. Also a low modulation current (270 mA) was used to decrease the rate of evaporation of liquid helium.

CHAPTER IV

RESULTS

The angular dependence of the frequencies of the fundamental dHvA terms for the field directions lying in the (110) plane is shown in Fig. 3. The various branches are labelled by the same Greek letters used by Mattheiss. In addition to six frequency branches, α, β, and γ_1^1 reported by Marcus, and γ_2, γ_3, γ_4 reported by Phillips and Shanks, we observed a frequency ($\gamma - \beta$) which changed from a value of 73.4 MG 15 degrees to [110] direction to 72. MG at the [110] direction. This is attributed to magnetic breakdown between γ and β Fermi surface sheets. The calculated frequency for this orbit is 8.3% greater than our measured value.

Cyclotron masses for the α, β and γ branches were determined for directions in the (110) plane. The mass was found from the least square fit of the slope of the l_n (Amplitude/Temperature) vs. temperature (eq. II-9). An example of the fit is shown in Fig. 4 for the effective mass of the α branch at 25.8° from the [001] direction. The cyclotron masses for the α, β and γ branches are tabulated in Table 1. The comparison of experimental data for the α , β and γ_1 branches with the mass values calculated by Mattheiss is shown in Fig. 5, 6 and 7. The α branch

resulted from the dominant oscillation throughout its (110) plane and it was well separated from the higher frequency branches. Thus, the mass of the α branch was easily measured. The mass values for this branch changes from a low of .574 m_0 at the [001] direction to a high of .72 m_0 near the [111] direction. For the β branch, the dHvA amplitude was maximum at the [001] direction, decreased gradually as the field direction went toward the [111] direction and increased again as the field approached the [110] direction. The dHvA signal for the β branch was weak near the [111] and mass measurements could not be done between 50 - 63° from the [001] direction. The mass values for the β branch varies from a low of .752 m_0 at the [001] direction to a high of .988 m_0 at the [111] direction. The oscillation for the γ_1, frequency had the smallest amplitude. The mass values for the γ_1 branch are .615 m_0 and .926 m_0 at [001] and [110] directions, respectively. At directions less than 16° from [110] direction, the β and γ_1, frequency branches are very close to each other and approximately 750 oscillations were recorded, to obtain enough resolution to separate them. In addition to these results, the mass value for the $\alpha - \beta$ frequency was determined, and was found to be 1.07 $\pm$ .02 M_0 at the [110] direction. This value is 20% higher than the value calculated by Mattheiss.

The experimental error of the measured effective masses

TABLE I

Direction (degrees from [001]	m^*/m α	m^*/m β	m^*/m γ
0.00 [001]	.574	.777	.615
2.00	.570	.752	.620
8.75	.585	.758	.648
10.50	.583	.783	.659
21.50	.633	.811	.698
25.75	.634	.823	.744
32.00	----	.841	.826
37.00	.652	.887	.857
44.50	.717	.988	.942
51.25	.72	.985	----
55.00 [111]	.694	----	----
58.00	.708	----	----
68.00	.70	.952	----
74.00	.71	.932	.982
80.00	.670	.922	----
84.50	.685	.920	.954
90.00 [110]	.687	.891	.926

FIG.3. dHvA frequencies of ReO_3 in (110) plane.

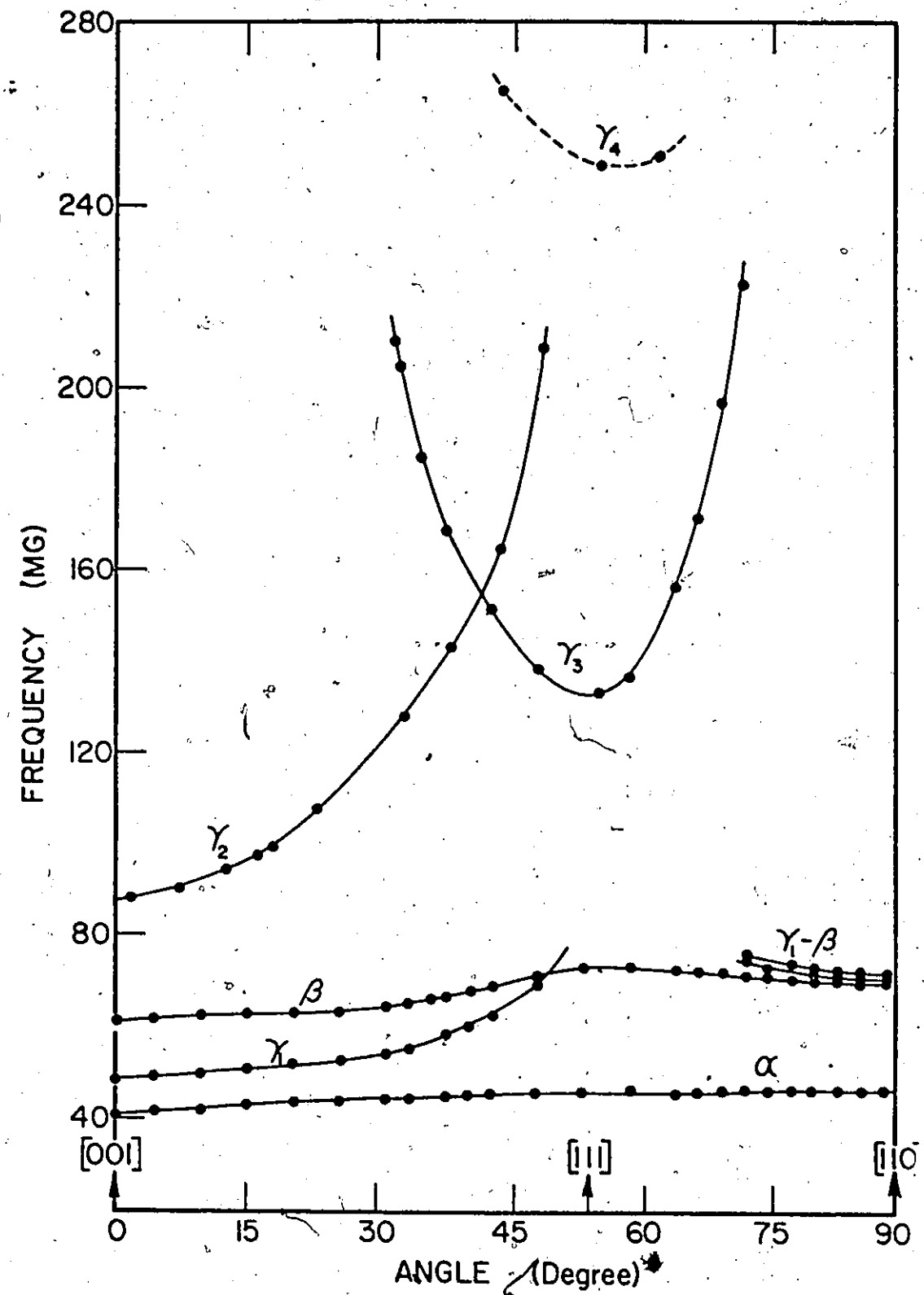
280
240
200
160
120
80
40
FREQUENCY (MG)
γ_4
γ_3
γ_2
$\gamma_1-\beta$
β
γ_1
α
[001]
[111]
[110]
0
15
30
45
60
75
90
ANGLE (Degree)

Figure 3

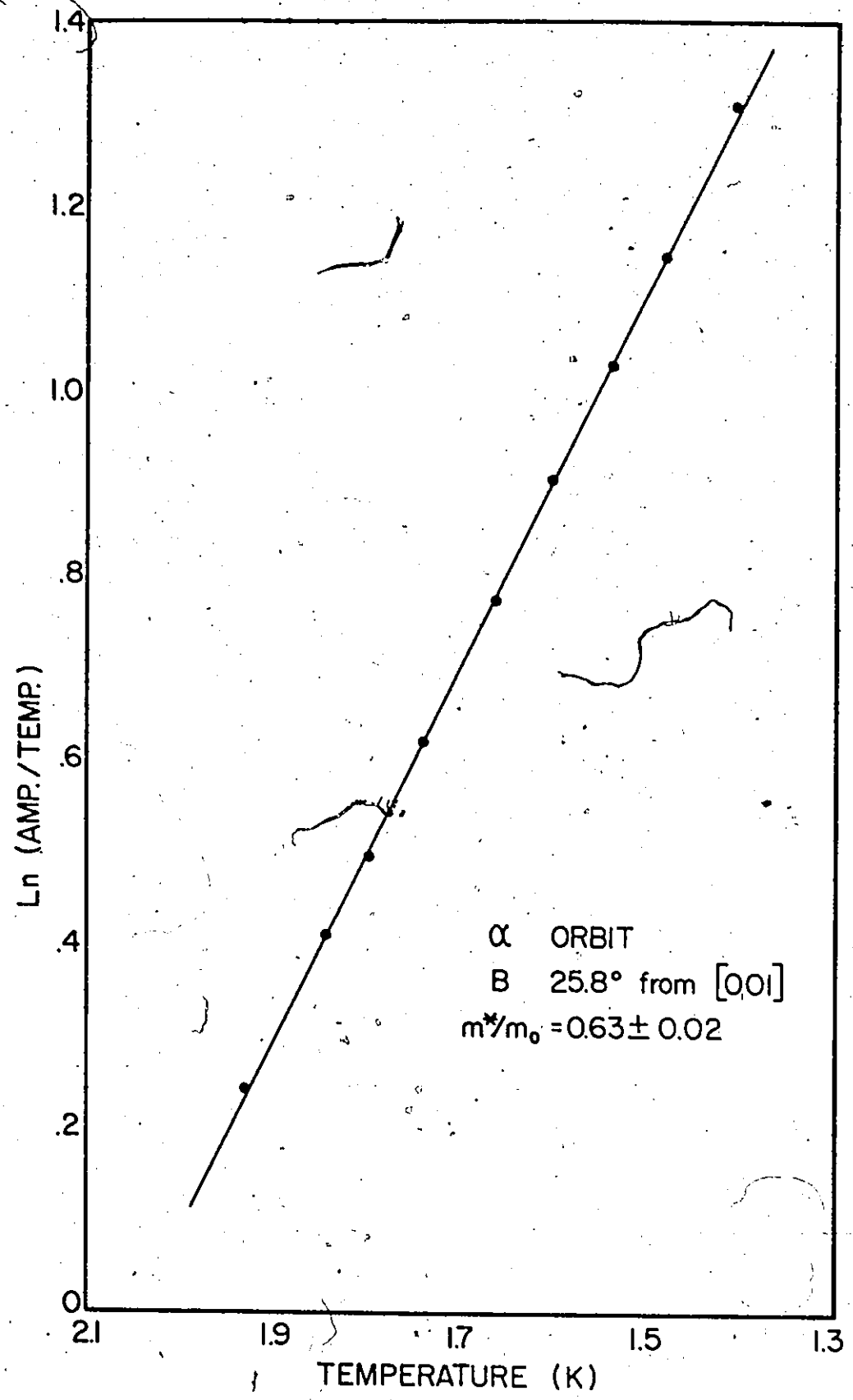
1.4
1.2
1.0
.8
.6
.4
.2
0
Ln (AMP./TEMP.)
2.1
1.9
1.7
1.5
1.3
TEMPERATURE (K)
α ORBIT
B 25.8° from [001]
m*/m₀ = 0.63 ± 0.02

Figure 4

FIG.5. Cyclotron mass for the alpha branch in the (110) plane.
Solid line: calculated by Mattheiss.

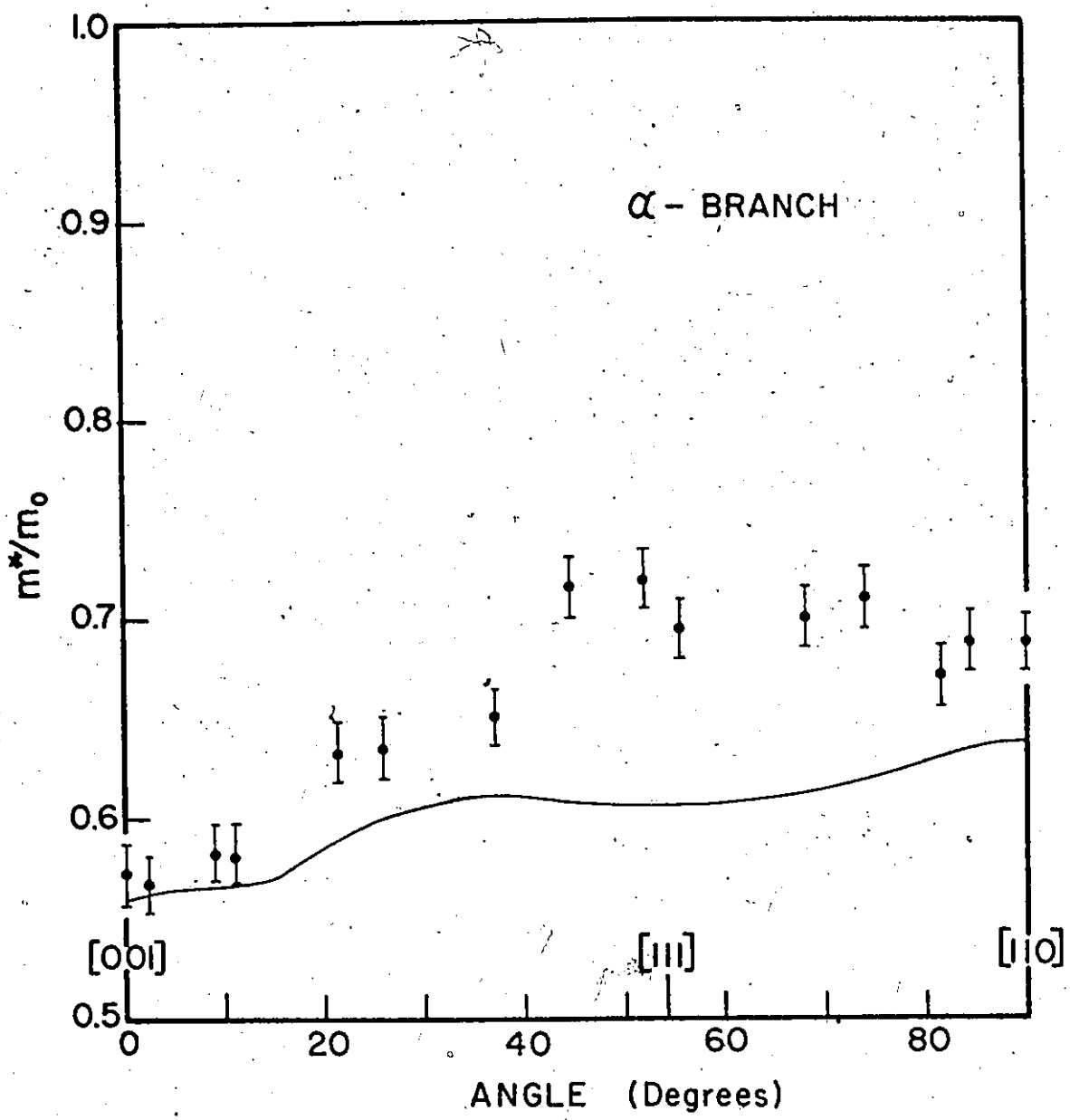
1.0
0.9
0.8
0.7
0.6
0.5
m*/m₀
α - BRANCH
[001]
[111]
[110]
0
20
40
60
80
ANGLE (Degrees)

Figure 5

FIG.6. Cyclotron mass for the beta branch in the (110) plane.
Solid line: calculated by Mattheiss.

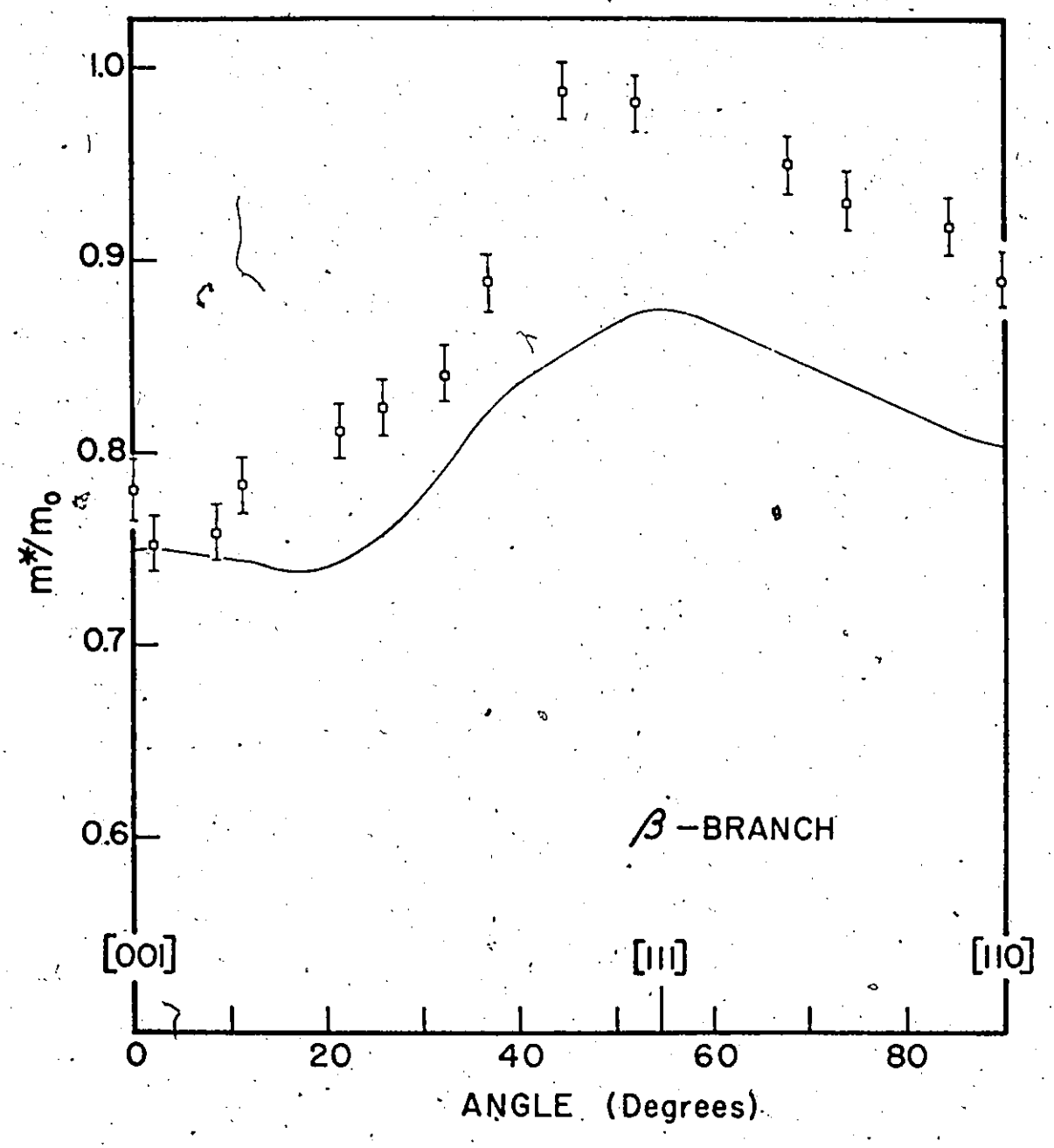
1.0
0.9
0.8
0.7
0.6
m*/m₀
β-BRANCH
[001]
[111]
[110]
0
20
40
60
80
ANGLE (Degrees)

Figure 6

FIG.7. Cyclotron mass for the gamma branch in the (110) plane.
Solid line: calculated by Mattheiss.

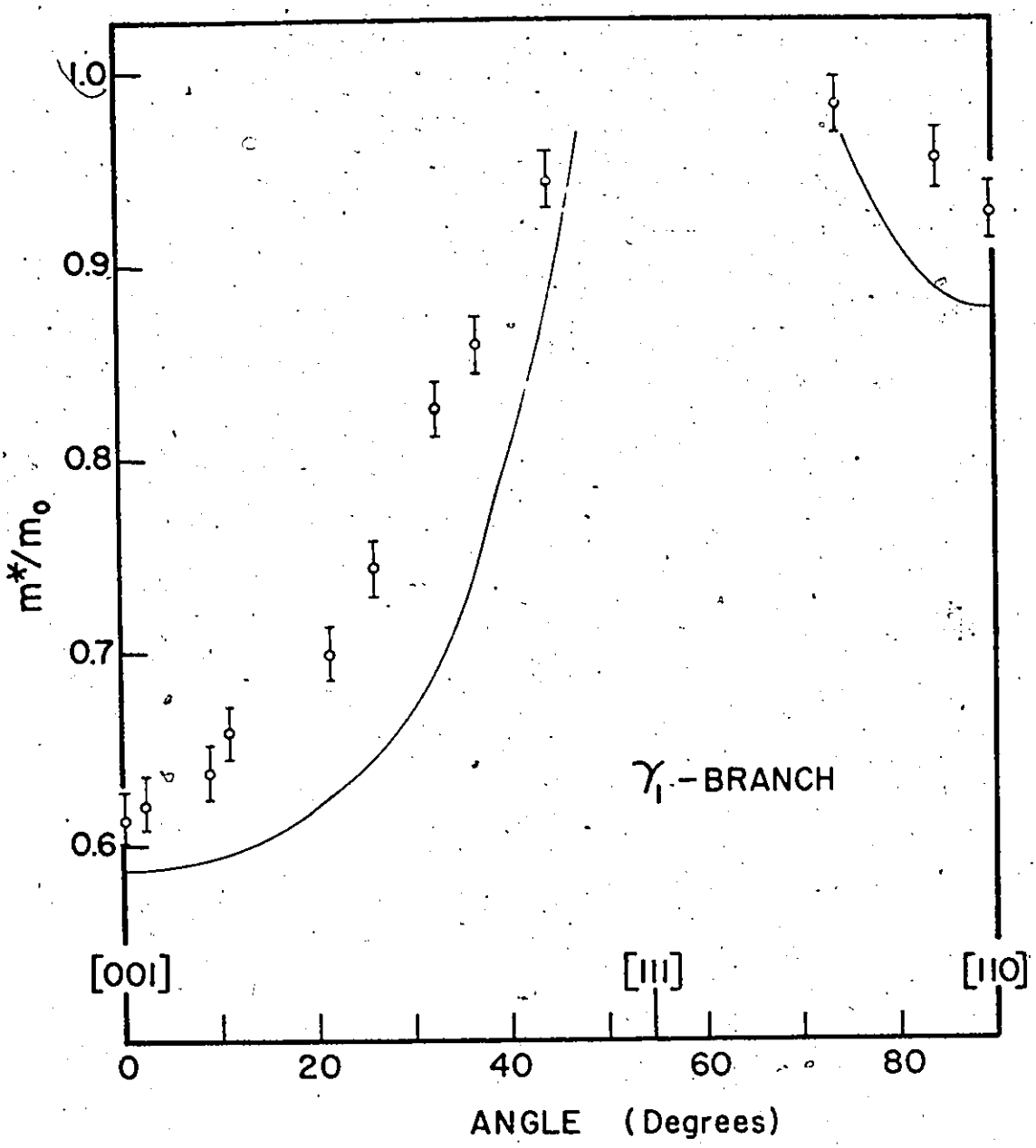
1.0
0.9
0.8
0.7
0.6
m*/m₀
γ₁ - BRANCH
[001]
[111]
[110]
0
20
40
60
80
ANGLE (Degrees)

Figure 7

was about 5%. The major source of error was due to measuring the dHvA amplitude from the Fourier transform peaks, which is an average over the magnetic field range. However, it was not possible to measure amplitude of one oscillation directly because several oscillation were always superimposed. Also the Fourier transform may not correspond exactly to the position of the dHvA frequency because of the digital nature of the computer analysis. There is also error due to temperature measurement and crystal misorientation.

If there is only one dHvA frequency such as for a metal with nearly spherical Fermi surface, the cyclotron mass can be measured to an accuracy of 1%. Also the same accuracy can be achieved by a system of parallel and perpendicular rotating modulation coils, so that one dHvA frequency can be singled out by filtering up to two dHvA frequencies from the spectrum (Windmiller 1966). This method was not applicable to the dHvA effect of ReO_3.

The Dingle temperature at the [111] direction of the α branch was found from the magnetic field variation of the dHvA amplitude at constant temperature. The Dingle temperature was determined from the least square fit of the slope of $\ln (A\sqrt{H}\ \mathrm{Sinh}\ (\alpha m^* T/H)/J_2(2\pi Fh/H^2))$ vs. H^{-1}. This is shown in Fig. 8, where F = 4635.6 Tesla is the dHvA frequency at the [111] direction for the α branch, and $m^* = .708\ m_0$. The Dingle temperature for this direction was found to be

$0.27 \pm .01$ k. This relatively small value of the Dingle temperature indicates that the crystal has a low density of dislocations.

FIG.8. Log plot used to determine the Dingle temperature T_D for the alpha branch at the [111] direction.

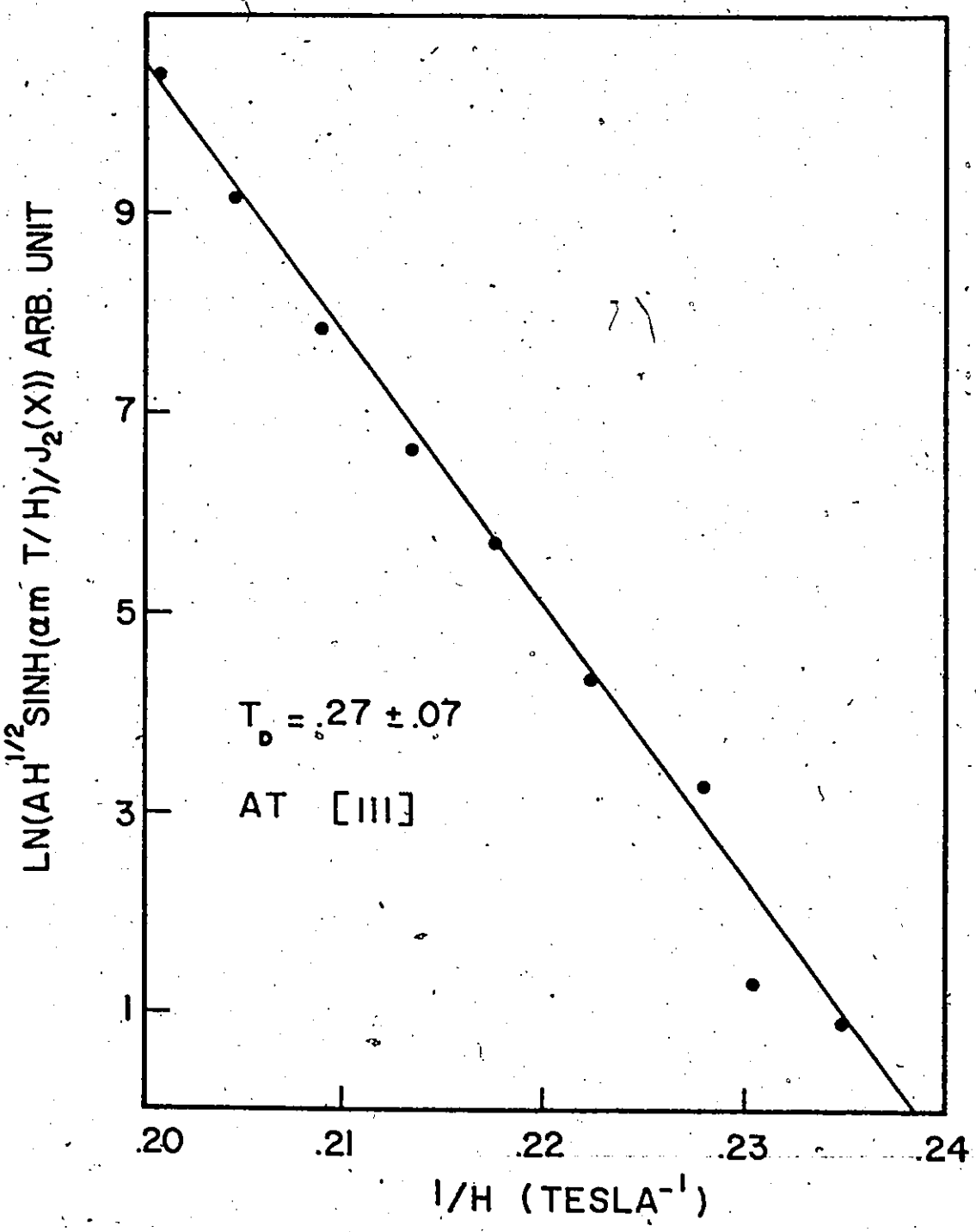
LN(AH^1/2 SINH(αm T/H)/J2(X)) ARB. UNIT
9
7
5
3
1
T_D = .27 ± .07
AT [111]
.20
.21
.22
.23
.24
1/H (TESLA^-1)

Figure 8

CHAPTER V

DISCUSSION AND CONCLUSION

The summary of comparison of this work for effective masses for α, β and γ branches with theory calculated by Mattheiss is shown in Fig. 9. The experimental results lie 2 - 15% higher than the calculated results.

Marcus has determined the cyclotron masses for the α sheet of the Fermi surface for three magnetic field directions. These are compared with our result in table II The cyclotron masses predicted by Mattheiss for the fitted and the adjusted band structure model of ReO_3 are also included in table II.

TABLE II

H	This Work	Marcus	Mattheiss Fitted	Mattheiss Adjusted
9° to [111]	.717	.68	.758	.637
at [111]	.695	.67	.757	.635
17 from [111]	.71	.65	.759	.645

The difference between this work and the fitted values of Mattheiss is about 6% whereas the difference between fitted theory and Marcus' data is twice as large. As mentioned previously, the discrepancy between the fitted results and

FIG.9. Comparison of experimental and calculated results for the three branches in the (110) plane.

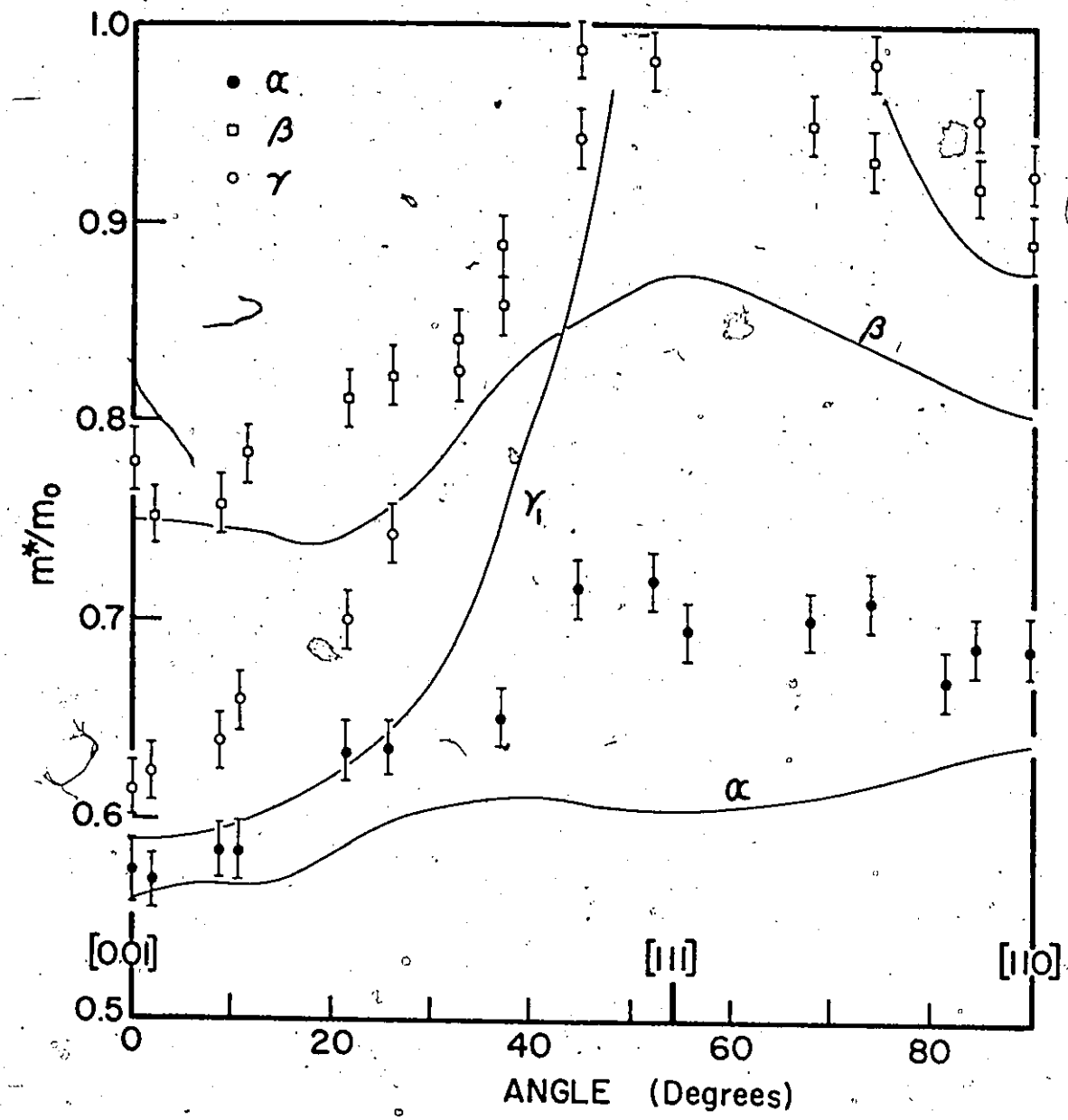
1.0
0.9
0.8
0.7
0.6
0.5
m*/m₀
α
β
γ
β
γ₁
α
[001]
[111]
[110]
0
20
40
60
80
ANGLE (Degrees)

Figure 9

the experimental values of Marcus was one of the factors which Mattheiss took into account to adjust his original APW band calculation. Our results show that the adjustment made by Mattheiss was an overcorrection because the mass values are less than those measured by Marcus.

As predicted by Mattheiss, a new frequency was observed having the frequency of 72MG and effective mass of 1.07 m_0 at the [110] direction. This frequency is about 8% lower and the effective mass is 20% higher than the corresponding calculated values. This frequency is attributed to the magnetic breakdown between the β and γ Fermi surface sheets. Experimentally, the magnetic breakdown behaviour could not be determined from the field dependence of the amplitude, because the dHvA signal together with that of β and γ disappear below 33. kO_e.

The band structure calculated by Mattheiss does not include electron-phonon interactions which contribute to the effective mass. The cyclotron mass measured in dHvA is increased by the electron-phonom interaction. Unfortunately the uncertainty in the calculated band structure mass is large enough that it is not possible to attribute any difference between the calculated and observed masses to electron phonon effects. However the close agreement (2-20%) between the calculated and observed mass indicates that the electron-phonon mass enhancement is not exceptionally large.

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