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# A STUDY OF THE FERMI SURFACES OF ANTIFERROMAGNETIC CHROMIUM-RICH ALLOYS USING THE DE HAAS-VAN ALPHEN EFFECT

by

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### INTRODUCTION

In an antiferromagnet, the magnetic moments are ordered in an antiparallel arrangement with zero net magnetic moment below a critical temperature, the Néel temperature,  $(T_N)$ . The antiferromagnetism of chromium, (Cr) has been studied extensively in recent years. The crystal structure of Cr and Cr-rich alloys is body-centered cubic (bcc). The magnetic moments at the cube corners are antiparallel but not equal in magnitude to those at the cube centers. The magnitude of the moments can be described by a spatially varying sinusoidal modulation called a spin density wave (SDW) with wave-vector  $\vec{q} = \frac{2\pi}{a}$  (1-3) ( $\hat{k}$ ), where  $\hat{k}$  is a unit vector along a cube axis (1). The repeat distance of the SDW is temperature dependent and varies between 21a and 27a (a is the lattice parameter and has the value 2.8765  $\stackrel{0}{A}$  at 0 K (2)).  $\delta$  depends on both temperature and alloy concentration. The term arises since the periodicity of the SDW differs from 2a and hence the wave-vector is somewhat less than one half of the smallest (100) reciprocal lattice vector, e.g.,  $\vec{G} = \frac{2\pi}{a}$  [002] (3). For temperatures greater than the Néel temperature there are no magnetic moments associated with the Cr atoms (4). Below the Néel temperature there is a second critical temperature called the spin-flip temperature  $(T_{SF})$  (1,5). For temperatures between  $T_N$  and  $T_{SF}$ , the polarization of the SDW is transverse; for temperatures below  $T_{SF}$  the polarization is longitudinal.

These experimental results are evidence for an itinerant electron model of the antiferromagnetism in Cr. In an itinerant antiferromagnet, the electron gas acts collectively to produce a spatially varying spin

density. Since the electrons in the electron gas are coupled only loosely to the Cr ions forming the bcc space lattice, the wave-vector of the SDW need not be connected with a reciprocal lattice vector. The SDW wavevector is the reciprocal lattice vector of a magnetic superlattice. The zone boundaries of the magnetic superlattice will produce energy discontinuities in the band structure similar to those produced by the Brillouin zone boundaries (6).

Studies have been done on the effects of alloying vanadium (V) and maganese (Mn) and other metals with Cr (1,7-16). The effect of alloying V with Cr is to decrease the Néel temperature and decrease  $\vec{q}$  while Mn has the opposite effect. Figure 1 shows the change in T<sub>N</sub> due to alloying V, Mn, and molybdenum (Mo) with Cr. As little as 4% V has the effect of reducing the Néel temperature from 312 K in pure Cr to less than 4 K in the alloy. This has been interpreted as arising from a modification of the Fermi surface (FS) of Cr due to alloying (1).

A model of the FS of Cr was first proposed by Lomer (17,18) who suggested the antiferromagnetism was due to flat pieces on the FS. Loucks (19) calculated the FS of paramagnetic Cr using an augmented-plane-wave (APW) method. A cross section for the (100) plane is shown in Figure 2. The following terms are used to describe the FS of Cr. The electron piece around  $\Gamma$  is the "electron jack." It has two parts--the "ball" surfaces and the "body." The hole surfaces at H are called the hole "octahedra." The small hole surfaces at N are the hole ellipsoids. In his calculations, Loucks did not find hole ellipsoids at N, although recent experimental evidence (20) indicates they are present. They are indicated by dashed



Figure 1. The change in Neel Temperature due to alloying V, Mn and Mo with Cr

Figure 2. Louck's calculation for the Fermi surface of Cr in a (100) plane. Experimental evidence indicates the presence of hole pockets at N although they are not present in Louck's calculations. The spin density wave vector  $\vec{q} = \frac{2\pi}{a}$  (1- $\delta$ ) [001] and  $\vec{q}^* = \frac{2\pi}{a}$  (1+ $\delta$ )[001] are also shown.

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lines in Figure 2. Lomer's model included these pieces but Loucks found in his calculation that they are sensitive to the potential used. It is seen that the body of the electron jack and hole octahedron are connected by  $\vec{q}_{*}$  Also shown in Figure 2 is  $\vec{q}^{*} = \vec{G} - \vec{q} = \frac{2\pi}{a}$   $(1 + \delta)$   $\hat{k}_{*}$ 

The interpretation of the change in the Néel temperature due to alloying is that the body of the electron jack and the hole octahedron are being modified to reduce the antiferromagnetic interaction (1). Because these two pieces tend to stabilize the SDW, changes in the antiferromagnetism of Cr will be primarily associated with these pieces. The hole ellipsoids and electron balls do not contribute to the formation of the antiferromagnetic state but are modified as a result of the antiferromagnetic interaction as will be discussed later.

Fedders and Martin (21) showed that the paramagnetic electron gas is stable to the formation of an antiferromagnetic state in the Hartree-Fock approximation when either Fermi-Thomas screening or dynamic screening is included. Antiferromagnetism in a metal is due to the band structure and FS, and in particular, to a pairing of electrons in different bands with different spins. The results of their calculation using a crude model for Cr are in agreement with experiment.

Since certain pieces of the FS are more important in the formation of the antiferromagnetic state, what happens to the pieces which do not participate as strongly in the interaction? Falicov and Zuckermann (6) investigated a Hamiltonian which had superlattice contributions to s-band terms and d-band terms and which neglected s-d hybridization. In the

Brillouin zone there are only s-d hybridized electrons. However, some pieces of the FS, e.g., the body of the electron jack and hole octahedron, are more d-like in character, while other pieces, e.g., the hole ellipsoids, are more s-like. The approximation made by Falicov and Zuckermann should be fairly good. They find energy gaps occur whenever  $\epsilon$  ( $\vec{k} + m\vec{G} + n\vec{q}$ ) =  $\vec{\epsilon}$  ( $\vec{k} + \vec{q}$ ), m and n are integers. The energy gaps occur at the Brillouin zone boundaries and at the magnetic zone boundaries. Since the wave-vectors,  $\vec{k}$ , all lie within the first Brillouin zone, the energy bands which have been remapped into the first zone are designated by m. The magnetic superlattice introduces energy gaps into each band at the intersection of the band and the magnetic zone boundaries. However, there will probably be magnetic breakdown of the energy gaps due to the magnetic interaction with  $n \ge 3$ . Only magnetic energy gaps with n = 1, 2seem to be important in interpreting de Haas-van Alphen (dHvA) data.

In the antiferromagnetic interaction large pieces of the body of the electron jack and hole octahedron are destroyed. Falicov and Zuckermann (6) ignore the portions of these surfaces which remain and consider only the ball surfaces and the hole ellipsoids. The superlattice introduces energy gaps in these surfaces and a whole new set of electron trajectories result. In particular, if  $\vec{q}$  is in the z direction, then pieces above the (001) plane are affected differently from those pieces in the (001) plane, Figure 3. The resulting FS pieces exhibit tetragonal symmetry. Figure 4 shows the bcc Brillouin zone with tetragonal notation. The truncation of the FS pieces due to the superlattice effects introduces new closed and open electron orbits (6).



Figure 3.  $\{100\}$  and  $\{110\}$  planes of the Fermi surface of Cr in the repeated zone scheme, assuming the hole octahedron and body of the electron jack are completely annihilated by the antiferromagnetic interaction. The dashed lines represent Fermi surface pieces translated by  $\pm \vec{q}$ .



Figure 4. The body-centered cubic Brillouin zone with tetragonal notation

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One method of examining the FS of a metal is the de Haas-van Alphen (dHvA) effect (22). In the dHvA effect, one observes oscillations in the magnetization of the electron gas which are periodic in 1/H, the reciprocal of the magnetic field. The frequency of these oscillations is related to the extremal cross sectional area of the FS by

$$f = \frac{e\hbar}{2\pi c} A_{ext} (\vec{k}) = K A_{ext} (\vec{k}) .$$
 (1)

dHvA measurements made on pure Cr crystals show tetragonal symmetry if the crystals have been previously field-cooled (23). Field-cooling refers to the fact that the crystal has been cooled through the Néel temperature in the presence of a large magnetic field. Magnetic susceptibility measurements showed that the magnetic state of the crystal depended on the magnetic field present when the temperature of the crystal was lowered below  $T_N$  (24). If the magnetic field,  $H_c$ , was 27 kilogauss and oriented along a  $\langle 100 \rangle$  direction, the magnetic structure could be described by a single  $\vec{q}$  parallel to  $\vec{H}_c$ , while for  $\vec{H}_c = 0$  there were three  $\vec{q}$ 's each parallel to a  $\langle 100 \rangle$  (25). dHvA measurements have shown the triple  $\vec{q}$  state to be a superposition of three sets of tetragonal data (one set for each  $\vec{q}$ ) (23).

Graebner and Marcus (20) have made a very extensive study of Cr using the dHvA effect. Figure 5 shows their dHvA data. They were able to interpret some of their data by considering truncations of the FS as described by Falicov and Zuckermann (6). The most convenient method of finding orbits which result from superlattice energy gaps is to translate a piece of FS, for example a hole ellipsoid at N<sub>2</sub>, by  $\pm \vec{q}$  (first order



Figure 5. dHvA frequency versus magnetic field direction for the major symmetry planes of Cr (20, p. 663)

transitions) or  $\pm 2\vec{q}$  (second order transitions). See Figures 3 and 6. Then a hole on the solid ellipsoid is allowed to make a first order transition to the dashed ellipsoid or a second order transition to the next solid ellipsoid. Graebner and Marcus (20) find agreement between the piece marked "a" in Figure 6 and frequency  $\zeta$  in Figure 5.

Since alloying V and Mn with Cr affects the antiferromagnetism in Cr as evidenced by changes in  $T_{N}$  and  $\vec{q}$  , dHvA measurements on Cr alloys should provide new insights into the effects the superlattice has on the FS. Optical measurements on Cr-alloys (26) have shown that for 0.94% Mn in Cr, the antiferromagnetism becomes commensurate with the lattice, i.e.,  $|\vec{q}| = \frac{1}{2} |\vec{G}| = \frac{2\pi}{a}$  and many of the energy gaps should disappear. When the antiferromagnetism becomes commensurate with the lattice the Brillouin zone changes to a simple cubic (sc) zone. Asano and Yamashita (27) have shown that the energy bands for the commensurate state can be approximated very well by remapping the energy bands of the paramagnetic state (bcc Brillouin zone) into a sc Brillouin zone. If one is able to observe dHvA signals in a commensurate crystal, these signals should be due to FS pieces found in the paramagnetic state of Cr. These pieces could be somewhat modified by the increased electron concentration and the change in symmetry from bcc to sc.

dHvA oscillations have been observed in several Cr-rich, Cr-V alloys with up to 2% V concentrations. Preliminary results for the frequencies obtained from these crystals have been reported (28).



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Figure 6. Method of constructing orbits for the hole ellipsoids at  $N_2$  in the (100) plane and for H parallel to [100]. Orbits from first order gaps are traced by following a dashed line and then a solid line; orbits for second gaps are traced by following either a solid line or a dashed line.

### EXPERIMENT

The dHvA samples were spark-cut from single or bi-crystal ingots grown in the Ames Laboratory by Mr. F. A. Schmidt (29). The nominal size of the samples used in the experiment were  $0.04^{11} \times 0.04^{11} \times 0.200^{11}$ . The samples were determined to be single crystals by X-ray diffraction techniques. With the exception of the 0.03% Mn sample, all the samples were cut with a (100) axis parallel to the long axis of the sample. The 0.03% Mn sample had a (112) axis parallel to the long sample axis. The alloy samples used in the experiment contained 2.0% V, 1.02% V, 0.58% V, 0.2% V, 0.09% V, 0.03% Mn, 0.04% Mn, 0.16% Mn and 0.91% Mn in Cr by weight. (Throughout the rest of the paper the % sign will be omitted.) There were also several samples with 0.45 Mn in Cr which back-reflection Laue photographs showed to be single crystals but in which no dHvA signals were observed. A possible explanation for the lack of dHvA signals was a concentration gradient in the samples.

The residual resistivity ratio (RRR) of the starting Cr material was approximately 300.<sup>\*</sup> In the 2.0V sample the RRR was approximately 11. The 0.1V, 0.2V, 0.03Mn, 0.04Mn, and pure Cr samples were annealed at 1150 C for 24 hours to remove strains.

The samples were mounted in a pick-up coil and this assembly was placed in a rotating-wheel sample holder. The sample was then oriented by X-ray diffraction techniques so that a (010) plane was perpendicular to the axle of the rotating wheel. All samples were oriented with the plane of

<sup>\*</sup>F. A. Schmidt, private communication.

rotation of the sample holder within 1/2% of a (010) crystal plane, except for the 0.03Mn sample which was oriented within  $1^{\circ}$  of a (110) crystal plane.

The sample holder, Figure 7, also contained a teflon and aluminum sample which was used to make nuclear magnetic resonance (NMR) measurements to calibrate the magnetic field. A modulation coil was then placed around the dHvA and NMR samples. This coil produced a small oscillating field so that the dHvA signal could be recovered from the noise using lock-in detection.

Figure 8 shows a block diagram of the apparatus which was assembled by Stone (30) and Boyle (31). The method used for measuring the dHvA signal is known as the field-modulation technique (32). Because of the non-linear nature of the magnetization of the sample, sidebands or harmonics of the modulating frequency were produced. The lock-in detector was adjusted to detect the second harmonic of the modulating frequency. The advantage of this in the present experiment was to discriminate against feed-through signals from the modulation coil in the first harmonic term which were larger than the dHvA oscillations. This allowed increased sensitivity in measuring the dHvA signals. In the case of the pure Cr sample the dHvA signal was approximately 2000  $\mu$  volts p-p at high fields while for the 2.0V and 0.9Mn samples the signals were on the order of 10 to 20  $\mu$  volts p-p.

The dHvA signal was amplified by the lock-in detector and then fed to a strip chart recorder and a voltage-to-frequency converter in the digitizing system. A sample of the oscillations for the 2.00 sample is shown in Figure 9. The oscillations were also recorded digitally on



Figure 7. An expanded view of the dHvA sample holder showing dHvA and NMR samples

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Figure 8. A block diagram of the dHvA apparatus



Figure 9. dHvA oscillations for the 2.0V sample. The field range is 48,231 gauss to 27,882 gauss.

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punched paper tape for computer analysis.

The magnetic field for the experiment was obtained from a Varian superconducting solenoid with a 1" bore and maximum field of 62 kilogauss. The field homogeneity was one part in  $10^4$  over a  $1 \text{ cm}^3$  sphere (31). The field was measured 5/8" above the sample by observing the NMR signal from fluorine or aluminum nuclei. At the NMR probe the field was approximately 6.4 gauss less than at the sample. The magnet was powered by a Varian X-4102 power supply. The supply had a motor driven 10-turn helipot which controlled the current and hence the magnetic field. This allowed the field to be linearly ramped up and down. The two ranges most commonly used for ramping were 50 and 100 minutes for 10 turns of the helipot.

The method of taking data was to set the NMR oscillator for some field near the starting point. The field was then either increased or decreased by the ramping mechanism in the power supply. When the field reached the setting of the NMR oscillator a signal appeared on an oscilloscope screen. As the signal moved across the center of the screen the digitizer was started and the field value recorded. After the field had swept through the appropriate range the NMR oscillator was set for a field value near the stopping point. When the NMR signal again crossed the center of the screen the digitizer was stopped and the field recorded. The ramping mechanism was then stopped. Using the oscilloscope to monitor the NMR signal, the field could be measured to  $\pm$  (7 to 15) gauss. This method of recording the data eliminates the non-linearity of the changing field at the starting or stopping points of the field sweep. For a more complete description of the sample holder and electronics, see the Ph.D. theses of

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Stone (30) and Boyle (31).

The samples were field-cooled after they had been aligned in the sample holder. In the case of the pure Cr, 0.1V, 0.2V, 0.03Mn and 0.04Mn samples, the sample holder and sample were heated above their respective Néel temperatures using an infra-red lamp. While the samples were heating, the magnet was set for a field in the range 40 to 50 kilogauss. The sample holder and sample were then quickly put into this field and allowed to cool below  $T_N$  with the field turned on. Typical cooling times were 30 to 60 minutes. The 0.5V, 1.0V, and 2.0V samples were put into the field without initial heating since  $T_N$  is below room temperature. An examination of the data showed the Cr and 0.1V samples and probably the 0.5V sample were field-cooled.

Because of the orientation of the samples, one  $\langle 100 \rangle$  axis was along the direction of maximum sensitivity of the pick-up coil while another  $\langle 100 \rangle$  axis was along the direction of minimum sensitivity. As a result, in the more concentrated alloy samples it was hard to observe dHvA signals in the direction of least sensitivity and thus hard to determine from the data if the samples were field-cooled. To counteract this problem, dHvA data was taken  $30^{\circ}$  away from each of the  $\langle 100 \rangle$  directions where the sensitivity of the pick-up coil was approximately the same. Then if the sample was field-cooled and had tetragonal magnetic symmetry, the dHvA oscillations would show different frequencies. If the sample was not field-cooled the two  $30^{\circ}$  directions would be equivalent and the dHvA frequencies would be the same for these two directions. The dHvA data for these two directions in the 0.5V sample were different and this forms the basis for saying the

sample was field-cooled. In the case of the 1.0V and 2.0V samples, no definite conclusions could be made, other than to say they were probably not field-cooled.

It has been proposed that a perfect crystal of Cr would show the tetragonal symmetry for  $H_c = 0$  (33). The converse of this is that  $H_c$  increases as crystal perfection decreases. In dHvA experiments the crystals usually have RRR approximately 1,000 to 50,000 and larger, and crystal purity is 99.99+% or better. Certainly alloy crystals with 1.0 to 2.0% impurity, while single, cannot be considered perfect crystals. Consequently, larger cooling fields are needed if they can be field-cooled at all. Therefore, it is surprising that any of the alloy samples could be field-cooled.

In the 2.0V and 0.91Mn samples, the dHvA oscillations were observed on top of another signal which had a parabolic dependence on time. It was determined from the field sweeps on the 0.91Mn crystal that this extra signal was due to the modulation field (which was proportional to  $H^2$ ) being picked up and not being rejected by the lock-in detector. While the signal was troublesome for the 2.0V data, it wasn't a serious problem. However, in the case of the 0.91Mn sample, the extra signal was serious since its range of amplitude was approximately constant while the dHvA signal decreased as the angle between  $\vec{H}$  and the axis of the pick-up coil (most sensitive direction) increased. After the electronics were checked and found to be operating properly, the cause of the problem seemed to be the amplitude of the first harmonic signal was larger than the amplitude of the second harmonic signal of the modulating frequency. The lock-in was not

able to reject completely the first harmonic signal.

The solution to the problem was to operate the lock-in detector on a less sensitive scale where the extra signal would not overload the amplifiers in the lock-in. The output of the lock-in was fed to an a-c coupled operational amplifier with a gain of 10. Compared to the dHvA signal, the extra signal was approximately d.c. and hence rejected by the operational amplifier, while the dHvA signal was amplified to a useable level. This method of recovering the dHvA signal worked well except for occasional noise spikes which the capacitively-coupled input circuit differentiated. The differentiated spikes overloaded the operational amplifier. Figure 10 shows a strip chart recording of the signal from the lock-in detector (a) and the signal after being amplified by the a-c coupled operational amplifier (b).

The digital data recorded on punched paper tape was converted to punched IBM cards for use as input to the computer program which Fourieranalyzed the data. Toward the end of the experiment the punched paper tape was recorded on 7-track magnetic tape by a machine in the Cyclone Computer Lab. A program (see Appendix) was written which read the 7-track tape, edited the data for output on punched cards and checked the data for digitizing errors. This program gave a listing of the data with the errors noted and a set of punched cards. The other alternative to punched cards was to analyze the data directly from magnetic tape. The extra programming and bookkeeping involved with data on magnetic tape and the relatively small number of punched cards from each date set did not warrant the change to magnetic tape.



Figure 10. dHvA oscillations in the 0.91Mn sample

(a) dHvA oscillations superimposed on parabolic signal. The change in magnitude of the extra signal is 1  $\mu$  volt while the maximum amplitude of the dHvA signal is 0.7  $\mu$  volt. (b) dHvA signal after amplification by a.c. coupled operational amplifier.

The errors involved in digitizing were due to the paper tape drive not advancing the paper tape and hence punching two characters on top of each other or else inserting an extra zero. Previous to the use of magnetic tape, each card was checked as it was being punched. The digitizer records each number as three digits with a minus sign associated with the highest order digit. The digits with the minus signs can only appear on the punched cards in columns equal to 1 modulo 3. A digit with a minus sign appearing in any other column meant there was a previous error.

The data were analyzed using a fast-Fourier subroutine RHARM. The method has been described by Cooley and Tukey (34). The advantage of using their method is the savings in computer time. Each analysis used three to four seconds of CPU (central processing unit) time.

For each crystal, ten or more field sweeps were made for  $\vec{H}$  parallel  $\vec{q}$  and for  $\vec{H}$  parallel [100] and perpendicular to  $\vec{q}$ . Frequencies which consistently appeared were averaged together and the average frequence recorded as being real for that crystal. The rms deviation for the averaged frequency was on the order of 0.5%. A plot was then made of dHvA frequencies against alloy concentration. The frequency spectrum for the dHvA oscillations for the 2.0V sample, Figure 9, is shown in Figure 11. For the 0.91Mn sample the dHvA frequencies were plotted against crystal direction.



Figure 11. dHvA frequency spectrum for the 2.0V data in Figure 9

#### RESULTS

Figure 12 shows the dHvA frequencies as a function of alloy concentration. The pure Cr, 0.1V and 0.5V samples are thought to be field-cooled and the frequencies for  $\vec{H}$  parallel to  $\vec{q}$  are indicated differently from the frequencies for  $\vec{H}$  perpendicular to  $\vec{q}$  and parallel to [100].

Figure 13 shows the change in three of the dHvA frequencies as a function of alloy concentration. These frequencies correspond to  $\zeta$  and  $\eta$  found by Graebner and Marcus (20), and arise from truncations of the hole ellipsoids at N<sub>2</sub> and N<sub>1</sub> by the magnetic superlattice. The dashed lines are the change in frequency of the truncated pieces. These frequencies were calculated using the dimensions for the hole ellipsoids determined by Graebner and Marcus (20). In the calculation, we assumed that alloying did not change the dimensions of the hole ellipsoids. The change in frequency of the truncated pieces was the result of a change in  $\vec{q}$  due to alloying. Since the calculated frequencies were smaller than the experimentally-measured frequencies for pure Cr would agree with the measured frequencies which have been renormalized so that the calculated and measured frequencies for pure Cr are the same.

Figures 14 and 15 show the dHvA frequencies as a function of crystal direction for the 0.91Mn crystal in the (010) and (110) planes. There seems to be a single frequency at 10.21 x  $10^6$  gauss which increases away from [001]. There are several frequencies around 18-20 x  $10^6$  gauss. These two regions are shown separately in Figures 16 and 17 for the (010) plane and in



Figure 12. dHvA frequencies versus alloy concentration. The data for pure Cr, 0.1V and 0.5V samples are indicated differently, since these samples are thought to be fieldcooled.

Figure 13. Three dHvA frequencies measured along [100] versus alloy concentration. The two frequencies  $\zeta$  are due to superlattice truncations of the hole ellipsoids at N<sub>2</sub>;  $\eta$  is due to superlattice truncations of the hole ellipsoids at N<sub>1</sub>. The dashed lines indicate the change in area due to a change in  $\vec{q}$  assuming the size of the ellipsoids does not change. The solid lines are the frequencies changes due to alloying with the calculated area normalized to the measured frequency in pure Cr. Points (a) and (b) are the calculated frequencies for pure Cr using the ellipsoid dimensions obtained from the 0.91Mn and 1.0V samples.





Figure 14. dHvA data as a function of crystal direction in the 0.91Mn sample for the (010) plane



Figure 15. dHvA data as a function of crystal direction in the 0.91Mn sample for the (110) plane

Figure 16. The low frequency region in Figure 14 drawn on an expanded scale. The solid lines represent the angular frequency variation of an hyperboloid of revolution.

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Figure 17. The high frequency region of Figure 14 drawn on an expanded scale. The solid lines represent the angular frequency variation of hole ellipsoids at M. The dashed lines are the angular frequency variation of electron ellipsoids of revolution at X. The boxed points represent the frequencies with the largest amplitude.



Figures 18 and 19 for the  $(1\overline{10})$  plane. The intensities of the frequencies starting at 10.21 x  $10^6$  are approximately 100 to 300 relative units. The frequencies in the range 18-20 x  $10^6$  vary between approximately 100 and 5,000 relative units, while the intensities of the frequencies around 22.8 x  $10^6$  were in the region 50 to 100 relative units. The frequency with the largest amplitude is shown by a boxed symbol.

The solid line in Figures 16 and 18 is the angular variation of the frequency which one would expect for an hyperboloid of revolution. As can be seen, there is reasonable agreement between the data and the curve.

Figures 17 and 19 show the higher frequency data on an expanded scale. The solid points are the frequencies which have the largest amplitude for a particular field sweep in a given direction. The solid lines are the calculated frequency variation for hole ellipsoids at M; the dashed lines are the calculated frequencies for electron ellipsoids of revolution at X. For the hole ellipsoids the frequencies 18.46, 19.37 and 22.87 x  $10^6$  gauss were used to determine the semi-axes of the ellipsoids. The calculated dimensions of the semi-axes are  $0.218 \text{ Å}^{-1}$ ,  $0.270 \text{ Å}^{-1}$ , and  $0.257 \text{ Å}^{-1}$  for the directions MH, MR and M $\Gamma$  respectively. Using these numbers, the curves were generated for both the (010) and (110) planes.

For the surfaces at X, we assumed an ellipsoid of revolution. The frequencies used to determine the semi-axes were 18.46, 18.46, and 20.44  $\times 10^{6}$  gauss. The semi-axes which were calculated were 0.225 Å<sup>-1</sup>, 0.249 Å<sup>-1</sup>, and 0.249 Å<sup>-1</sup> for the directions Xr, XM, and XR respectively.

Some other frequencies with comparable amplitudes to those near the calculated lines were observed. These frequencies are also shown on the

Figure 18. The low frequency region in Figure 15 drawn on an expanded scale. The solid lines represent the angular frequency variation of an hyperboloid of revolution.

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Figure 19. The high frequency region of Figure 15 drawn on an expanded scale. The solid lines represent the angular frequency variation of hole ellipsoids at M. The dashed lines are the angular frequency variation of electron ellipsoids of revolution at X. The boxed points represent the frequencies with the largest amplitude.



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figures but we have no explanation for them. One possibility is the resolution of the Fourier analysis is too high. As will be explained later, the uncertainty in the frequency or half-width of the peak is on the order of 1/N, where N is the number of cycles. If there are 100 cycles, the resolution is about 1%. However, if the analysis tries to resolve the peak frequency to 0.5%, the 1% wide peak splits up into a series of peaks. The result is that several frequencies are recorded instead of just one frequency. However, several of the field sweeps were analyzed using a filter-periodogram method with reduced resolution and these extra points were indicated as being present but not resolved as actual peak frequencies in the spectrum. The filter-periodogram method analyzes the data by first filtering the data using a digital filter. The filtered data is then analyzed by a periodogram technique. The advantage of first filtering the data is to reduce large sideband frequencies associated with the periodogram analysis (35).

We feel the precision of the frequencies which were measured was on the order of 0.2%. Since the frequencies were determined based on the number of cycles present in each data set, there was an uncertainty in each frequency due to the Uncertainty Principle. This uncertainty was given by (100/N)%, where N is the number of cycles in the data set. We tried to use a field sweep large enough to get at least 200 cycles of the high frequencies, i.e., in the range 18-20 x  $10^6$  gauss. This means there was an uncertainty of 0.5% for this frequency range and a 1% uncertainty for the lower frequency region.

For the high frequency region there could be a 1% resolution for some

of the frequencies. This happens if frequency A + 0.5% overlaps frequency B - 0.5%. The Fourier routine can then only resolve the two frequencies to 1%. To get 0.5% resolution one would need approximately 400 cycles of each frequency or 0.25% resolution. Since the signals are weak at low fields this would mean extending the field sweep range at the high end which is not possible with the present magnet. The 0.5% and 1.0% error bars are indicated for a frequency of 20.0 x 10<sup>6</sup> gauss.

# DISCUSSION

Since all the alloy samples were not field-cooled, all the data were plotted on one graph and examined for trends. The frequency variation of the two branches  $\zeta$  with alloy concentration can be followed. Since there were no extra frequencies near  $\zeta$  for  $\overline{H}$  perpendicular to  $\overline{q}$  and parallel to [100] in pure Cr, it was assumed that in the alloys this would also be true. Hence all the points near the calculated lines in Figure 12 can be associated with the two  $\zeta$  branches as shown in Figure 13.

When V or Mn are added to Cr, relatively large changes are observed in  $T_N$  and  $\vec{q}$ . One possible interpretation of this is that the addition of V or Mn acts to increase or decrease the number of 3d electrons in the crystal. This follows since the d-like surfaces, the hole octahedron and body of the electron jack, seem to be responsible for stabilizing the antiferromagnetic state.

As a first approximation in trying to explain the frequency change of  $\zeta$  we assumed the hole ellipsoids would not be affected by alloying. The only effect alloying has then is to change the magnitude of  $\vec{q}$  and hence change the point of truncation of the hole ellipsoids. See Figures 3 and 6. Using the dimensions  $0.173 \ A^{-1}$ ,  $0.234 \ A^{-1}$ , and  $0.268 \ A^{-1}$  for the semiaxes of the ellipsoids along the directions NH, NT, and NP (20) respectively, and the values of  $\vec{q}$  for the different alloys (13) the areas and frequencies for the  $\zeta$  branches in the alloys were calculated. The conversion factor 104.8 (K of Equation 1) was used to convert area in  $A^{-2}$  to frequencies in  $10^6$  yauss. This is shown by the dotted lines in Figure 13. The calculated

areas were then normalized to the experimentally determined frequencies for pure Cr. The normalizing factors were 109.3 for the lower branch of the  $\zeta$ frequency, and 110.6 for the higher branch of the  $\zeta$  frequency. This shift of approximately 5% gives good agreement with the data.

There is also a second set of hole ellipsoids at the points  $N_1$ . The frequency changes of the truncated pieces of these ellipsoids due to the variation of  $\vec{q}$  with alloying were calculated. These frequencies are shown by the dotted line rear T in Figure 13. Again the calculated area was normalized to the experimental value for pure Cr. The normalizing factor had the value 109.7. The calculated curve passes through observed dHvA frequencies, but except for the data points for 0.1V, 0.5V, and pure Cr, the other data points could be due to frequencies which would be observed for  $\vec{H}$  parallel to  $\vec{q}$  had the crystals been field-cooled.

Assuming that the only effect of alloying V or Mn with Cr is to change the magnitude of  $\vec{q}$  and not the size of the hole surfaces at N, a consistent interpretation of the data results. The normalizing factors are within 1% of each other and have the effect of increasing the calculated frequencies on the order of 5% to agree with experiment. There are several possibilities which could explain the discrepancy.

The first possibility is that the dimensions of the ellipsoids which were used to calculate the cross-sectional areas are too small. Graebner and Marcus report the dimensions for the hole ellipsoids as those which best fit their data and "...slightly different shapes were found to give worse agreement with the data" (20. p. 668). The implication is that the areas they calculated for the truncated pieces differed from the

experimentally-measured frequency, also. The data for the two c branches and frequency n from the present study for pure Cr agree with those obtained by Graebner and Marcus (20). Since the present data is for only one crystallographic direction, the data cannot be used to determine the dimensions of the hole ellipsoids independently.

Another possibility is that the sharp edges of the second order truncated FS pieces, Figure 6, are rounded by second order interactions at the plane of intersection of the two hole ellipsoids. Two second order intersecting ellipsoids are shown in Figure 20a. At the point of intersection (A) the bands could be as shown in Figure 20b. The magnetic interaction due to the magnetic potential  $V_{M}(\vec{K},\vec{q})$  at the point,  $|\vec{K}_{F}| =$  $|\vec{k}_{F} + 2\vec{q}|$  causes the bands to mix and split apart. The result is two new FS points: one of which is on the closed FS piece in Figure 6 while the other is on the open FS piece in Figure 6.

For directions in k-space near the intersection point, the energy bands will also be affected by the magnetic interaction. Near the magnetic superzone boundaries, energy gaps will occur as shown in Figure 20c. Depending on the relative position of the Fermi energy  $(E_F)$  and the energy gap, the Fermi wave-vector  $(k_F)$  can either increase, decrease or remain the same. Two different values of  $E_F$  in Figure 2<sup>0</sup>c illustrate the first two cases. Since the relative position of  $E_F$  and the energy gap need not be the same for all directions in k-space,  $k_F$  can increase, decrease or remain unchanged near the intersection point of the two ellipsoids. It is also possible for  $E_F$  to lie in the energy gap. In which case the FS point disappears. This case is not of interest in this discussion since a closed

Figure 20. Second order interaction of the hole ellipsoids at  $N_2$ 

- (a) Second order intersection of two hole ellipsoids at  $N_{2}$
- (b) Two energy bands for the two hole ellipsoids at the point A. Mixing of the energy bands could cause them to split as shown giving rise to a point on the closed orbit Fermi surface piece (a) in Figure 6 and a point on the open orbit Fermi surface in Figure 6.
- (c) The effect on the Fermi wave vector due to the relative position of the Fermi energy,  $E_F$ , with respect to the superlattice energy gaps at the magnetic zone boundary for point B. For  $E_F$  above the energy gap  $(E_{F_1})$ ,  $k_{F_{after}} > k_{F_{before}}$ ; for  $E_F$  below the energy gap  $(E_{F_2})$ ,  $k_{F_{after}} < k_{F_{before}}$ .



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ENERGY (arb. units)

FS piece is assumed to exist after the magnetic interaction. As the direction in k-space moves further away from the intersection point, A, the energy gap moves further away from the Fermi level (either up or down) and the intersection point of the energy band and Fermi level is affected less by the magnetic interaction.

As a result of these considerations, the area of the truncated FS piece can either increase in magnitude, remain the same or decrease in magnitude. Without a detailed knowledge of the band structure along many directions in k-space and a good approximation for the magnetic interaction potential, a definite theoretical conclusion cannot be reached. The experimental data indicate the areas of the truncated pieces increase in size.

Either of the explanations or a combination of both can be used to justify increasing the calculated frequencies 5% to make them agree with the experimentally measured frequencies for pure Cr. This shift then gives consistent results for the calculated and measured frequencies in the alloys, assuming that the hole ellipsoids are not affected by alloying and only  $\vec{q}$ changes with alloying.

Optical data has shown that approximately 0.9Mn in Cr produces a commensurate antiferromagnet (26). When the antiferromagnetism becomes commensurate with the lattice, the magnetic superlattice has simple cubic symmetry. Asano and Yamashita have calculated the band structure for Cr assuming the antiferromagnetism is in a commensurate state (27). The results of their calculations are similar to what one would obtain by remapping the paramagnetic Cr bands from a bcc Brillouin zone into a simple

cubic Brillouin zone. The Fermi surface which they calculated is shown by dashed lines in Figure 21. The feature to be noticed is that there are hole pockets at M and a small hole piece between  $\Gamma$  and X. The hole piece along  $\Gamma X$  is part of the hole octahedron which remains after the antiferromagnetic interaction occurs. There are also two electron pockets at X.

The high frequency angular data from the 0.91Mn crystal were fitted to an ellipsoid of revolution and a regular ellipsoid. These surfaces were tentatively identified as due to the small electron piece at X and the hole ellipsoid at M, respectively.

As can be seen from Figure 17, the stronger signals correspond to the ellipsoid of revolution. In the (010) plane the agreement between an ellipsoid of revolution and the strong signals is quite good. However, in the (110) plane, Figure 19, the strong signals do not fit an ellipsoid of revolution.

In the (010) plane much of the data were fitted to a regular ellipsoid. The agreement between the calculated curves and the data points is quite good. In the ( $\overline{110}$ ) plane the strong signals seem to have the same angular dependence as a regular ellipsoid. The largest deviation occurs at  $30^{\circ}$ from [001] toward [110] and is about 2%.

One possible explanation for this is that the crystal was misaligned in the magnetic field and was rotating in some plane other than  $(1\overline{10})$ . If this were the case, the strong signals as well as the others belong to the hole ellipsoids in both the (010) and (1\overline{10}) planes. Several families of curves for misalignments of 5<sup>°</sup> in several directions were calculated. The curves showed the crystal could have been misaligned, but by an amount

greater than  $5^{\circ}$  (on the order of  $10^{\circ}$ ). However, curves for a  $10^{\circ}$  misalignment would fit the strongest data points but not many of the other data points. The curves for a  $5^{\circ}$  misalignment fit very few of the data points, irrespective of intensity.

An argument against misalignment can be made. X-ray diffraction photographs taken before and after the data runs showed that the crystal was oriented in the sample holder to less than  $0.5^{\circ}$  away from either the (010) or (110) plane of rotation. It is true that the X-ray pictures show the relative orientation of the sample and sample holder with respect to the X-ray beam. The sample could be misaligned  $5^{\circ}$  in one direction and the sample holder  $5^{\circ}$  in the opposite direction so the misalignments cancel and the crystal appears to be perfectly aligned. Another possibility is the sample holder isn't positioned properly in the magnet, so that the direction of  $\vec{H}$  is not in the plane of rotation of the sample holder.

In the experiment, all of the dHvA samples were aligned in the sample holder in exactly the same way and the sample holder was positioned in the magnet in the same orientation for all of the data runs. If either the crystal was misaligned or the field vector was not in the plane of rotation, then the data for all the crystals would be for some direction other than a  $\langle 100 \rangle$  direction. In the case of the alloys, there is no way of deciding this. However, for pure Cr one could decide by comparing our data to that of Graebner and Marcus (20). In particular, they find frequency  $\mu$  along  $\vec{q}$ ([001]) has the value 15.6 x 10<sup>6</sup> gauss and frequency  $\mu$ <sup>1</sup> has the value 16.0 x 10<sup>6</sup> gauss. At an orientation of approximately 13<sup>°</sup> from  $\vec{q}$  in a (010) plane, these frequencies are the same and have the value 16.2 x 10<sup>6</sup> gauss. Since these values are minimum for this direction, a misalignment would tend to increase these two frequencies. For the same direction in our field-cooled Cr crystal, we measure these frequencies as  $15.59 \times 10^6$  gauss and  $16.01 \times 10^6$  gauss. We feel that misalignment of the 0.91%Mn crystal is not a problem.

Another possibility for the strong intensity frequencies not lying on the regular ellipsoid curves in the  $(1\overline{10})$  plane is that the ellipsoids in the 0.91Mn crystal are distorted in the  $(1\overline{10})$  plane with maximum distortion occurring  $30^{\circ}$  from [001] toward [110]. However, if this were the case one could expect to see effects of the distortion occurring in the (010) plane also.

The dimensions we obtained in the 0.91Mn sample for the semi-axes of the hole ellipsoids are 0.218  $A^{-1}$ , 0.257  $A^{-1}$ , and 0.270  $A^{-1}$  along the lines MH, MT, and MR, respectively. Assuming the small electron piece at X to be an ellipsoid of revolution, we obtain the dimension 0.225  $A^{-1}$  for the XT direction and 0.249  $A^{-1}$  perpendicular to the line XT. (The point H is in a bcc Brillouin zone and is equivalent to the point T in a sc Brillouin zone.) The dimensions are shown in Figure 21 along with the FS for pure Cr determined by Asano and Yamashita (27). Our hole ellipsoid at M is smaller than the calculated value while the smaller of the electron pockets at X is larger than the calculated value.

There was also a lower frequency signal observed in the 0.91Mn sample. The angular dependence of this signal is shown in Figure 16 for the (010) plane and Figure 18 for the ( $\overline{110}$ ) plane. The solid line in Figure 16 is the angular variation of an hyperboloid of revolution fitted to the frequencies at [001] and [101]. In Figure 18 the solid line is a hyperboloid



Figure 21. The calculated Fermi surface of Cr in the commensurate antiferromagnetic state determined by Asano and Yamashita is indicated by dashed lines. The Fermi surface determined from the data for the 0.91Mn sample is shown by the solid lines.

of revolution fitted to the frequencies at [001] and 40<sup>0</sup> from [001] toward [110]. The strength of the signals are approximately 100 relative units around [001] where the sensitivity of the pick up coil is greatest. It could not be determined conclusively if the signal could be followed through 90°. As the sample is rotated away from [001] the frequency increases but the strength decreases and is on the order of 25 relative units at [100] (Figure 16). Since the commensurate crystal is expected to have cubic symmetry, if the  $10.21 \times 10^6$  gauss frequency at [001] continuously increases through  $90^{\circ}$  of rotation, there should then be a higher frequency signal at [001] which continually decreases to  $10.21 \times 10^6$  gauss through 90° of rotation. We do find a weak signal (approximately 50 units in intensity) at [001] with frequency around 17 x  $10^6$  gauss, and there is a comparable signal at [100]. The problem is that if this signal is weak along the direction of maximum sensitivity then it will be weaker still along the direction of least sensitivity. As a result we cannot claim with any certainty that this signal exists through a  $90^{\circ}$  interval away from [001]. We tentatively identify this signal as being associated with the portion of the hole octahedron remaining after the antiferromagnetic interaction occurs. The circular cross-sectional dimension is indicated in Figure 21.

Recent optical data of Bos and Lynch (26) on Cr-Mn alloys was interpreted using the assumption that the hole pockets at M are not present. They see an absorption peak in the 0.94Mn and higher concentration crystals and associate this with the loss of the hole pockets due to the additional electrons filling the hole pocket energy bands.

The present data for the lower concentration V and Mn alloys can be interpreted by assuming that alloying has little effect on the s-like pieces of FS and a large effect on the d-like pieces. For the larger concentration of V and Mn some departure from this behavior is expected. The dimensions for the hole ellipsoids in the 0.91Mn sample are larger than the corresponding dimensions in pure Cr except along the MR (or NP) lines in the two samples respectively. An indication that alloying 1% V in Cr has an effect on the size of the hole ellipsoids at N can be seen in Figure 13 for frequency  $\eta_{\bullet}$  The calculated frequency (assuming that alloying doesn't change the size of the hole ellipsoids) is 30% larger than the experimental frequency of 4.50 x 10<sup>6</sup> gauss in the 1.0V sample. An explanation for the 30% difference between the calculated and experimental frequencies is that the hole ellipsoids are becoming smaller when large concentrations of V are alloyed with Cr.

Using the dimensions obtained in the present study for the hole ellipsoids in the 0.91Mn sample, the calculated frequency (using the normalizing factor 109.7) for  $\eta$  in pure Cr is 20% larger than the experimental value. A frequency for  $\eta$  in pure Cr can also be calculated from the 1.0V sample data using one assumption. It is necessary at this point to explain the method used for calculating the area of the truncated ellipsoid at N<sub>1</sub>, Figure 3. Figure 22 is an enlarged drawing showing the truncated area and relative orientation of the semiaxes with respect to the (100) plane (the measuring plane for  $\vec{H}$  parallel to [100]). The truncated area, A, is given

by

$$A = 2 \left[ \frac{bx_2^{'}}{\ell} \sqrt{\ell^2 - x_2^{'2}} + \ell b \sin^{-1} \frac{x_1^{'}}{\ell} - 2\delta x_2^{'} \right]$$
(2)

Figure 22. Truncation of the hole ellipsoids at  $N_{j}$  due to the magnetic superlattice

- (a) The truncated area (projected in the (100) plane) of the hole ellipsoids at  $N_1$  due to second order superlattice effects is shown by the striped lines.  $X_1^i$  is the point of intersection of the hole ellipsoids.
- (b) Relative orientation of the Nr, NH lines with respect to the x-axis and the semi-monor axis & viewed in the (100) plane.

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where  $x_2^1$  is the intersection point of the two ellipsoids in the (100) plane, b is the dimension along NP,  $\delta$  is defined by  $|\vec{q}| = \frac{2\pi}{a} (1 - \delta)$ and  $\ell$  is the dimension along the direction  $\Gamma$ H and is equal to

$$\ell = \sqrt{\frac{2(N_{\Gamma})^{2}(N_{H})^{2}}{(N_{\Gamma})^{2} + (N_{H})^{2}}}$$
 (3)

 $(N\Gamma)$  and (NH) represent the dimensions along the directions  $N\Gamma$  and NH respectively. The frequencies calculated for pure Cr based on the 0.91Mn and 1.0V data are indicated by (a) and (b) in Figure 13.

Since the dimension along MR in the 0.91Mn sample is the same as the equivalent dimension in pure Cr (i.e., along the NP direction), it is assumed in the following that this dimension is the same in the 1.0V sample. Then & can be adjusted so that the calculated area for the truncated piece agrees with the experimental area for the 1.0V sample. The truncated area can then be calculated for pure Cr. The calculated frequency (using 109.7 as the normalizing factor) is found to be 20% lower than the experimental frequency in pure Cr.

The argument is a self-consistent one. Since Mn has the effect of increasing the electron concentration by one electron per atom while V decreases the electron concentration by the same amount, it might be expected that Mn and V should have equal and opposite effects, neglecting lattice changes due to the different sizes of the V, Cr, and Mn ions. Noticing that one dimension of the hole ellipsoids remains the same for 0.91Mn in Cr, then it is expected that this dimension will be the same for 1.0V in Cr. Based on this assumption, it is possible to determine  $\xi$ .

from the 1.0V data. The truncated area and frequency calculated for pure Cr are 20% lower than the experimental frequency. This is the opposite effect to adding 0.91Mn since in that case the calculated area and frequency are 20% larger than the experimental frequency for pure Cr. Since the dimensions for the hole ellipsoids in the 0.91Mn sample are larger than the corresponding dimensions in pure Cr (except along the lines MR and NP in the two samples, respectively) and a consistent interpretation shows the dimensions in the 1.0V sample to be smaller than in pure Cr (except along the line NP), then it appears that the rigid band theorem is not applicable to the smaller FS pieces in pure Cr.

In the rigid band model, the energy bands are allowed to shift without changing shape and different bands are allowed to shift differently. Changing the electron-to-atom (e/a) ratio has the effect of shifting the Fermi energy relative to the bottom of each band. Increasing e/a shifts the Fermi level up relative to the bottom of the band while decreasing the number of electrons has the opposite effect. Neutron diffraction and resistivity studies (13) on the magnetic properties (principally  $T_N$  and  $\vec{q}$ ) of ternary Cr-V-Mn alloys have shown that the rigid band theorem is applicable to the pieces of the FS (the hole octahedron and body of the electron jack) which contribute mainly to these properties. These studies do not, however, allow one to reach a conclusion as to the effect alloying has on other pieces of the FS such as the hole ellipsoids.

The properties which were measured related to the magnetic state of the Cr alloys. As has been shown, these properties are most influenced by the d-like FS pieces, the body of the electron jack and hole octahedron.

If this is true, then adding V or Mn to Cr has the principal effect of changing the number of d-like electrons. Applying the rigid band theorem to the d-bands gives agreement with experiment.

Applying the rigid band theorem to the whole FS, one would expect the hole pieces to decrease in size and the electron pieces to increase in size. The present results show that the smaller electron piece around X does increase in size. The problem arises when one considers the hole pieces at M. The present measurements in the 0.91Mn crystal indicate these pieces are larger than those in pure Cr, while a self-consistent argument for the 1.0V crystal shows these pieces are smaller than those in pure Cr, contrary to what the rigid band theorem predicts. Bos and Lynch (26) assumed the rigid band theorem in interpreting an absorption peak due to the filling of the hole pockets.

The dimension associated with the frequency of 10.21 x 10<sup>6</sup> gauss is tentatively identified with the remaining piece of the hole octahedron after the magnetic interaction. This dimension is larger than the calculated value. The calculated piece could be increased in size if the body of the electron jack and hole octahedron do not nest as perfectly as Asano and Yamashita (27) obtain in their calculation. Using the rigid band theorem, we would expect this piece to be somewhat larger in pure Cr than it is in the 0.91Mn crystal. However, in pure Cr this piece probably would not be observed because the magnetic superlattice would have an effect on this surface similar to the effects on the hole ellipsoid surfaces.

The rigid band theorem seems to be applicable to the d-bands in Cr

and the FS pieces associated with these bands. The dimensions which we measure for the 0.91Mn crystal are larger than the corresponding dimensions for pure Cr. Since one would expect, on the basis of a rigid band picture, that the hole pieces in the 0.91Mn should be smaller, the rigid band theorem applied to the whole FS of Cr is not applicable. Bos and Lynch (26) state that their interpretation of their optical data is not consistent with the FS determined by Asano and Yamashita (27). The interpretation of the data from the present study is consistent with these FS calculations. Even allowing for misalignments of the crystal or magnetic field (as discussed previously), the data is consistent with regular ellipsoids at M. Misalignments could account for the dHvA signals which are attributed to the ellipsoids of revolution at X. The interpretation of the present data then is not consistent with the interpretation of the optical data of Bos and Lynch (26), but is consistent with the FS calculations of Asano and Yamashita (27). The study also argues against applying the rigid band theorem to the s-like pieces of the FS of Cr.

### CONCLUSIONS

We have shown that in the more dilute alloys the change in dHvA frequencies can be associated with a change of  $\vec{q}$ . By assuming that alloying small concentrations of V and Mn in Cr doesn't affect the size of the hole ellipsoids, the change in areas of the truncated FS pieces is due only to a change of  $\vec{q}$ . Our data are in good agreement with this assumption. The data for the 0.91Mn and 1.0V show the rigid band picture is not applicable to the smaller FS pieces.

In the commensurate sample (0.91Mn), a more detailed study which includes data in several other high symmetry planes and at intervals smaller than  $10^{\circ}$  would lead to a more precise picture of the FS. Also, examining the FS in a more concentrated crystal, approximately 1.5% to 2.0% Mn, would give a better test of the rigid band theorem as applied to the small FS pieces. One would also be able to determine if there are signals in the 18 to 20 x  $10^{\circ}$  gauss region which arise from two different pieces of the FS or if they are due to misorientation of the crystal. It would also be possible to measure the distortion, if any, of the hole ellipsoids.

The difficulty of using higher concentration alloy crystals is the reduction of signal strength. This can be overcome partly by using larger magnetic fields, which could be obtained in a pulsed-field dHvA experiment. In the 0.91Mn sample, these larger fields would allow one to measure the larger electron surface at X.

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# APPENDIX

This appendix gives a brief description of the computer programs used in analyzing the data. Job C334AZZZ, "TAPE TO CARD CONVERSION", read the 7-track tape produced in the Cyclone Computer Lab from the punched paper tape, punched the data on IBM cards and printed a listing of each data set. C334AYYY, "CARD FIXUP", corrected bad data sets by either inserting or deleting a character and produced a new set of punched cards and listing for the data set. C334AEJG is the program which analyzed the dHvA data.

The analysis program has two options: the data can be analyzed using a filter periodogram technique described by Panousis (35) or the data can be analyzed using the Fast Fourier subroutine RHARM. Both options have been checked using both test data and real data. There is more resolution in the Fourier option for a reasonable size of memory space. Increasing the amount of memory improves the resolution of the filter-periodogram method until it is comparable to the resolution obtained from RHARM.

The MAIN part of the program reads a title card with a parameter specifying the analysis option. The subroutine STEADF reads a card containing the NMR frequencies corresponding to the starting and stopping field values and converts the frequencies to magnetic fields in gauss. It then reads the data cards and converts the three digit numeric numbers to machine numbers. Subroutine STEAD1 converts the data from points evenly spaced in H to points evenly spaced in 1/H. This is necessary since the dHvA oscillations are periodic and sinusoidal only in 1/H. Control of the program then returns to MAIN.

If the data is to be analyzed using the filter-periodogram technique, FILTER is then called and the frequency spectrum computed. For the Fourier analysis, RHARM is called and the Fourier coefficients are computed. The coefficients which are computed correspond to the number of cycles which fit in the data set, e.g., the coefficients  $a_1$  and  $b_1$  correspond to one cycle in the data set. a is the cosine coefficient and b the sine coefficient. The intensity of a frequency (equal to  $a_i^2 + b_i^2$ ) is then computed.

Subroutine FIT then searches the results of either analysis for peaks in the frequency spectrum and fits a second order curve to determine the true peak frequency. These frequencies along with their intensities are printed out.

MAIN then calls a graphing routine, GRAPH, if desired, and the frequency spectrum is plotted. The program is then ready to analyze the next data set.

When using RHARM, care must be taken to see that the proper coefficients are squared and added together, i.e.,  $(a_i^2 + b_i^2)$  instead of  $b_i^2 + a_{i+1}^2$ ). The index i is generated by the formula

$$i = 2x \frac{(first frequency of interest)}{\begin{vmatrix} \frac{1}{H} & -\frac{1}{H} \end{vmatrix}} + 1$$
  
final start

so that the initial value of i is always odd. Boyle (31) noticed a splitting of the peaks at higher frequencies. An examination of his program showed that he did not compute the index so that the initial value of i was odd. As a result he could sometimes use  $(b_i^2 + a_{i+1}^2)$  instead of the correct term  $(a_i^2 + b_i^2)$  in determining his frequencies. Using test data, a frequency shift was observed if i was not odd. If two frequencies were close together, so that they were not completely resolved, then using  $(b_i^2 + a_{i+1}^2)$  would lead to a splitting which would appear not to be real.

The amplitude of the dHvA signal is a function of H, and is largest at large fields. The increasing amplitude doesn't affect the frequency of the peak. This was checked by using test data of constant amplitude and also test data with a 3 : I amplitude variation from high fields to low fields. A provision was added to generate constant amplitude real data by increasing the amplitude at low fields. Again the real frequencies, i.e., those with large intensities, occur at the same value, while the noise shifts slightly.

Finally the program was run in WATFIV to check for any programming errors such as parameters in subroutines not having the same character as those in the CALL statement. The other possible error of interest was too many values generated for an array. A few minor errors of this type were found and corrected.

The listing of the three programs, including control cards, follows.

```
//C334AZZZ JOB ACC26.SIZE=128K.TIME=3.GUTMAN
            EXEC PL1LFCG, PARM. PL1L= "DPT=2, DECK", REGION. GD=128K
//$1
//PL1L.SYSIN DD *
 /* TAPE TO CARD CONVERSION */
 /*
    THIS PROGRAM READS THE 7-TRACK TAPE CONTAINING THE DATA INTO A 100
  ELEMENT ARRAY WITH 78 CHARACTERS PER ELEMENT AND CHECKS THAT THE TOTAL
 NUMBER OF CHARACTERS = 0.0 MODULO 3. THE PROGRAM THEN CHECKS EACH
  ELEMENT FOR LETTERS (NEGATIVE NUMBERS) IN LOCATIONS 1 MODULO 3.
  IF IT FINDS LETTERS IN OTHER LOCATIONS, IT LISTS THOSE LOCATIONS.
 THE PROGRAM THEN LISTS THE ELEMENTS AND PUNCHES CARDS (1 CARD PER
  ELEMENT).
                                                                     */
 MAIN:
         PROC OPTIONS (MAIN);
         DCL EN FILE INPUT SEQUENTIAL;
         DCL CARDS CHAR (7800) VARYING;
         DCL OUT CHAR (80):
         DCL O (80) CHAR (1) DEFINED OUT UNALIGNED:
         DCL BCARD CHAR (80);
         DCL CDSZ FIXED BINARY (31,0);
         DCL FBUF CHAR (7800);
         DCL BUF (100) CHAR (78) DEFINED FBUF UNALIGNED;
         ON ENDFILE (EN) GO TO FINISH;
         ON ERROR BEGIN;
           KODE = ONCODE:
                              ON CODE = ', KODE (A(18), F(10, 0))
           PUT EDIT ('ERROR
             (*NUMBER OF RECORDS READ = *, NREC) (X(20), A(25), F(10, 0))
             SKIP(4);
         END:
         BCARD = (80) 'A';
         CDSZ = 78;
         NREC = 0;
         PUT EDIT ('STARTING TO READ TAPE') (A(21)) SKIP(4):
         OPEN FILE (EN):
 START:
         READ FILE (EN) INTO (CARDS);
         NREC = NREC + 1;
         K = LENGTH (CARDS);
         J = MOD (K,3);
```

```
FBUF = CARDS;
        KP = K / CDSZ;
        KPP = MOD (K, CDSZ);
        IF KPP > 0 THEN KP = KP + 1;
        ELSE;
        PUT PAGE EDIT (K, KP) (2 F(6,0));
        PUT FILE (PUNCH) EDIT (BCARD) (A(80));
        IF J > 0
          THEN DO;
            PUT LIST ('DATA SET IS BAD');
          END;
          ELSE;
CHEKIT:
            DO I = 1 TO KP BY 1;
            OUT = BUF(I);
            IND = 0;
            INDP = 0;
              DO N = 2 TO CDSZ BY 3;
              IF O(N) =  • THEN DO;
                N = CDSZ;
                GO TO SKPCHK;
                END;
              IF O(N) < "0" THEN IND = N;
              ELSE IF O(N+1) < O' THEN IND = N+1;
              ELSE:
              IF IND > 0
                THEN DO;
                IF INDP = 0
                  THEN DO:
                  PUT EDIT (**ERROR IN COLS.*) (A(15)) SKIP;
                  END;
                PUT EDIT (IND) (F(4,0));
                INDP = 1;
                I \cdot ND = 0;
                END;
              ELSE;
SKF'CHK:
              END;
            PUT EDIT (DUT) (A(80)) SKIP;
PRINTIT:
```
```
PUT FILE (PUNCH) EDIT (OUT) (A(80));

END;

GO TO START;

FINISH: PUT EDIT ('FINISHED READING TAPE. NUMBER OF RECORDS = ',NREC)

(A(44),F(7,0)) SKIP(4);

END MAIN;

//G().PUNCH DD SYSOUT=B,DCB=(RECFM=FB,LRECL=80,BLKSIZE=80C)

//G().EN DD UNIT=(TAPE7,,DEFER),VOLUME=SER=TPO132,LABEL=(1,NL),
```

```
// DISP=(OLD,KEEP),DCB=(DEN=1,TRTCH=ET,RECFM=U,BLKSIZE=7800)
```

```
//C334AYYY JOB 40026,TIME=3,SIZE=128K',GUTMAN
         EXEC PL1LFCG, PARM.PL1L='DECK, OPT=2', REGION.GO=128K
//S1
//PLIL.SYSIN DD *
 /* CARD FIXUP */
 /*
     THIS PROGRAM READS IN A DATA SET FROM CARDS AND THEN ADDS OR
 DELETES CHARACTERS.
       NCD =NUMBER OF CARDS IN DATA SET.
       NCHS =NUMBER OF CHANGES.
       NCDN(J) = NUMBER OF THE CARD TO BE CHANGED.
       NCOL(J) = COLUMN NUMBER ON CARD TO BE CHANGED. TO ADD A CHARA-
         CTER, MAKE THIS A NEGATIVE NUMBER.
       KARA(J) = CHARACTER TO BE INSERTED (IF ANY).
                                                                       */
 MAIN:
         PROC OPTIONS (MAIN);
         DCL ( BUF (100) CHAR (80),
             TEMP1 CHAR (80),
             TEMP2 CHAR (80),
             BLANK CHAR (80),
             DUT CHAR (80).
             NCOL(9),
             NCDN(9),
             KARA (9) CHAR (1),
             CDSZ FIXED BINARY (31,0) ) STATIC;
         DCL 01 (80) CHAR (1) DEFINED TEMP1 UNALIGNED;
         DCL 02 (80) CHAR (1) DEFINED TEMP2 UNALIGNED;
         CDSZ = 78;
         BLANK = (80) • •:
 START: BUF = BLANK;
         GET EDIT (NCD, NCHS, (NCDN(J), NCOL(J), KARA(J) DO J = 1 TO 9),
           IMD) (2 F(3,0), 2 F(3,0), X(1), A(1), 2 F(3,0), X(1), A(1),
           2 F(3,0), X(1), A(1), 2 F(3,0), X(1), A(1), 2 F(3,0), X(1), A(1),
           2 F(3,0), X(1), A(1), 2 F(3,0), X(1), A(1), 2 F(3,0), X(1), A(1),
           2 F(3,0),X(1),A(1),F(2,0));
         IF NCD < O THEN STOP;
         ELSE:
    GET EDIT ((BUF(I) DO I = 1 \text{ TO NCD}) (A(80)):
       DO M = 1 TO NCHS:
```

```
MP = NCDN(M);
 MPP = MP + 1;
IF NCOL(M) > 0 THEN DO;
TEMP1 = BUF (MP);
TEMP2 = BUF(MP+1);
 DO I = NCOL(M) TO CDSZ;
   O1(I) = O1(I+1);
 END;
 O1(CDSZ) = O2(1);
 BUF(MP) = TEMP1;
TEMP1 = TEMP2;
 DO J = MPP TO NCD;
  TEMP2 = BUF(J+1);
  DO K = 1 TO CDSZ;
     O1(K) = O1(K+1);
   END:
   O1(CDSZ) = O2(1);
   BUF(J) = TEMP1;
   TEMP1 = TEMP2;
 END;
END;
ELSE DO;
 KOL = -NCOL(M) + 1;
 TEMP1 = BUF(NCD);
 DO J = NCD TO MPP BY -1;
  TEMP2 = BUF(J-1);
  DO K = CDSZ TO 2 BY -1;
     O1(K) = O1(K-1);
   END;
   01(1) = 02(CDSZ);
   BUF(J) = TEMP1;
   TEMP1 = TEMP2;
 END:
 DO I = CDSZ TO KOL BY -1;
  O1(I) = O1(I-1);
                     •
 END;
 O1(KOL-1) = KARA(M);
```

```
BUF(MP) = TEMP1;

END;

END;

PUT PAGE;

DO L = 1 TO NCD;

OUT = BUF(L);

PUT EDIT (OUT) (A(80)) SKIP;

PUT EDIT (OUT) (A(80));

END;

GO TO START;

END;

//GO.PUNCH DD SYSOUT=B,DCB=(RECFM=FB,LRECL=80,BLKSIZE=800)

//GO.SYSIN DD *

DATA
```

```
-1
```

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```
//S1
         EXEC FORTG, REGION.GO=128K, TIME.GO=03, LINES=5
//FORT.SYSIN DD *
С
С
      THIS PROGRAM ANALYSES LINEARLY-RAMPED MODULATED-FIELD DE HAAS-
С
      VAN ALPHEN DATA BY MEANS OF FREQUENCY FILTER RESPONSE SYNTHESIS.
С
      FOLLOWED BY PERIODOGRAM ANALYSIS.
      A PROVISION HAS ALSO BEEN ADDED TO ANALYZE THE DATA BY A FAST
С
С
      FOURIER FIT. RHARM.
      THE FREQUENCIES AND RELATIVE INTENSITIES ARE PLOTTED AND PRINTED.
С
С
С
      GUTMAN
                ACCOUNT A0026 CRYSTAL PHYSICS VII, AMES LAB.
                                                                ISU
С
С
      THIS IS THE MAIN PROGRAM.
С
С
      THE DIMENSION STATEMENTS BELOW ALLOW FOR 200 FILTER PASSFREQUENCIES
С
      (UU), 200 FILTER INTENSITIES (ZZ), AND 200 PERIODOGRAM INTENSITIES
С
             SPACE IS ALSO ALLOTED FOR 100 FILTER RESPONSE MAXIMA (UU2, Z2)
      (Z).
С
      AND 100 PERIODOGRAM RESPONSE MAXIMA (UU1.Z1).
C
      DOUBLE PRECISION DRH, FACTOR
      DIMENSION UU1(100), Z1(100), UU2(100), Z2(100), Z(200), ZZ(200)
      DIMENSION UU(200)
      DIMENSION HEAD(10)
      DIMENSION ARRAYT(7)
      DIMENSION XLAB1(5), YLAB1(5), GLAB1(5), GLAB2(5)
       COMMON XLAB(5),YLAB(5),Y( 8200),INV(2100),S(2100)
      KS=3
      IMIN=1
      LMAX=0
      OUTRA=10.**30
С
      THE FIRST CARD IN THE DATA GIVES AXIS LABELS FOR GRAPHING THE
С
      INPUT DATA. THIS IS THE ONLY TIME THIS SET OF LABELS IS READ IN,
C.
      EVEN FOR MORE THAN ONE DATA SET.
      READ (1,6) XLAB, YLAB, XLAB1, YLAB1
    6 FORMAT (20A4)
    ] FORMAT (2F5.0,3F6.0,2F4.0,2I2,10A4)
```

74

```
DE HAAS-VAN ALPHEN COMPUTATIONS-- DATA SET NUMBER
  2 FORMAT ("1
  1,12A4)
                 RATE=",F4.0," KCPS.
  3 FORMAT (*O
                                      HSCALE=",F6.4,"
                                                           HZERO=",F6.0
                                      COILK=',F6.0,' GAUSS/VOLT TZE
   1, GAUSS THETA= F7.2, DEG.
   1RO=",F4.0," MSEC.")
    ON THE SECOND CARD, CONTROL NUMBERS AND LABELS FOR THE DATA SET ARE READ.
    RATE=-1 FOR THIS PROGRAM. HSCALE, TZERO, NADD USUALLY ARE NOT USED.
    HZERO SPECIFIES THE FERROMAGNETIC INTERNAL FIELD (OR SOLENOID OFFSET),
    THETA SPECIFIES THE FIELD ROTATION ANGLE FOR FERROMAGNETS.
    QQQ IS THE FILTER Q (SET BY PROGRAM TO 10 IF NOT SPECIFIED).
    HEAD IS THE DATA SET LABEL (40 SPACES ALLOTED).
     IF NADD<0 THE FAST FOURIER FIT WILL BE USED
     IF KREP<0 FREQUENCY RANGES WILL BE READ IN AFTER THE DATA HAS
     BEEN FOURIER ANALYZED.
 4. READ (1,1) RATE, HSCALE, HZERO, THETA, COILK, TZERO, QQQ, KREP, NADD,
  1(HEAD(I), I=1, 10)
  5 WRITE (3,2) (HEAD(I), I=1,10)
 9 DO 8 I=1,5
    GLAB1(I) = HEAD(I)
  & GLAB2(I)=HEAD(I+5)
    DELT=0.0
    CALL STARTM(DELT)
    DO 7 I=1,8200
 i^{*} Y(I)=0.
    HSCALE=HSCALE/10000.
    THETA=THETA/100.
    WRITE (3,3) RATE, HSCALE, HZERO, THETA, COILK, TZERO
    PIE=3.14159
    TZERO = TZERO / (10.**6)
    THETA=THETA*PIE/180.
    NDEG=3
    IF (QQQ) 731,731,732
731. 000=10.
732 CONTINUE
```

```
CALL DATE(ARRAYT)
      WRITE (3,103) ARRAYT
  103 FORMAT (4X, 7A4)
  100 CONTINUE
  200 CONTINUE
  30() CALL STEADF (QQQ,MPTS,DRH,H1,THETA,HZERO,HEAD,FFIRST,FLAST,RES,
     ITIMEM, KMAX, NPTS
  400 CONTINUE
      RES1=RES*100.
  601 FORMAT ('O
                        LOWEST FREQUENCY CONSIDERED WAS = . E10.3)
                        HIGHEST FREQUENCY CONSIDERED WAS =', E10.3)
  602 FORMAT (
                                                          =', F6.3,'
                        RESOLUTION
  603 FORMAT ( •
     1PERCENT!)
  606 FORMAT ( 
                                                          =', F3.0)
                        THE FILTER Q
С
С
      THE CONTROL NUMBERS 'NFIRST' AND 'NLAST' ARE SET UP. NFIRST IS THE NUMBER
С
      OF POINTS PER CYCLE OF FFIRST THAT THE DATA CONTAIN. NCOL IS EQUAL TO
С
      THE NUMBER OF POINTS PER CYCLE OF THE FILTER PASSFREQUENCY.
      THE BASIS FOR THE PERIODOGRAM IS BEING SET UP HERE.
                                                              FFIRST AND FLAST
С
      ARE REDEFINED SO THAT EXACTLY NFIRST AND NLAST POINTS PER CYCLE OF EACH
С
                 NSTEP IS ROUGHLY PROPORTIONAL TO RES AND TO NLAST (TO AVOID
С
      EXIST.
      MORE THAN 200 PASSES THROUGH THE FILTER) AND HAS AN ABSOLUTE VALUE OF
С
      AT LEAST 1. MORE PASSES THROUGH THE FILTER THAN THE NUMBER SET UP HERE
С
С
      CAN BE DONE BY REDUCING RES OR BY INCREASING NPTS AT THE START.
С
      IF(NADD.LT.0) GO TO 1461
      NFIRST=1./(DRH*FFIRST)
      FFIRST=1./(DRH*NFIRST)
      NLAST=1./(DRH*FLAST)
      FLAST=1./(DRH*NLAST)
      NSTEP=1+NLAST*RES
                                    NFIRST=", I6, " NLAST="I6, " NSP", I3)
   32 FORMAT ('O
                    DRH=",E10.3,"
      WRITE (3,32) DRH, NFIRST, NLAST, NSTEP
  608 NCOL=NFIRST
      UO=2.*PIE*FFIRST
      WRITE (3,601) FFIRST
      WRITE (3,602) FLAST
```

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```
605 WRITE (3,606) QQQ
     WRITE (3,603) RES1
      IF (NFIRST .GT. 1000) GO TO 424
     I = 1
 305 CALL FILTER (DUT, IMIN, NPTS, DRH, UO, QQQ, NCDL, KMAX, OUT2)
     IF (OUT-OUTRA) 690,690,691
 691 WRITE (3,692)
 GO TO 307
 690 Z(I)=OUT
     ZZ(I)=OUT2
     UU(I)=UO/(2.*PIE)
     IF (I-200) 725,725,824
 824 WRITE (3,825)
 GO TO 307
 725 I=I+1
     NCOL AND UO ARE CHANGED, AND THE FILTER IS AGAIN CALLED.
C
     NCOL=NCOL-NSTEP
     UO=2.*PIE/(DRH*NCOL)
  11 IF (NCOL-NLAST) 307,305,305
 307 CONTINUE
     LLL=I-1
     CALL FIT (LLL,ZZ,UU,UU2,Z2,RATIO,LK2)
 101 FORMAT (61X, END OF FILTER FIT.")
     WRITE (3,101)
     CALL FIT (LLL,Z,UU,UU1,Z1,RATION,LK)
     THE FILTER SPECTRUM IS ADJUSTED TO BE PLACED IN A LOWER GRAPH.
С
     DO 1010 I=1.LLL
1010 ZZ(I) = ZZ(I) - 1.
     DO 427 I=1,LK2
 427 Z2(I) = Z2(I) / RATIO
 428 WRITE (3,415) RATION
     WRITE (3,1000) RATIO
 415 FORMAT ('
                     NORMALIZING FACTOR (PERIODOGRAM) = . E10.3)
 1000 FORMAT (*
                     NORMALIZING FACTOR (FILTER)
                                                   =",E10.3)
     IF (MPTS) 430,426,426
```

```
426 CONTINUE
      THE PERIODOGRAM SPECTRUM IS GRAPHED.
С
      CALL GRAPH (LLL, UU, Z, KS, 3, 12, 10, 0, 0, 0, 0, 2, -1, 0, XLAB1, YLAB1,
     1GLAB1.GLAB2)
     THE FILTER SPECTRUM IS GRAPHED.
С
 431 CALL GRAPH (LLL, UU, ZZ, KS, 3, 0., 10., 0, 0, 0.2, -1.0, 0, 0, 0, 0)
  430 WRITE (3,416)
  416 FORMAT ('0')
С
      THE FILTER MAXIMA ARE PRINTED OUT.
      WRITE (3,1001)
                        FILTER ANALYSIS!)
 1001 FORMAT ('0
      WRITE (3,417)
                                                             INTE
  417 FORMAT( 0
                     FREQUENCY
                                            NORM. INTENSITY
     1NSITY!)
       WRITE(3,416)
      DO 1005 I=1.LK2
 1005 WRITE (3,1006) UU2(I),Z2(I)
 1006 FORMAT(E18.5.E25.5)
       WRITE(3,416)
      DO 418 I=1.LK
       ZZ(I)=Z1(I)
  418 Z1(I) = Z1(I) / RATION
      THE PERIODOGRAM MAXIMA ARE PRINTED, USING A NOISE LEVEL OF 0.005.
С
 1002 FORMAT ( • 0
                          PERIODOGRAM ANALYSIS!)
      WRITE (3,1002)
      WRITE (3,417)
       WRITE(3,416)
       DO 820 I=1,LK
       IF(Z1(I)-0.005)820,420,420
  420 WRITE(3,421) UU1(I),Z1(I),ZZ(I)
  421 FORMAT(E18.5,E25.5,E19.5)
  820 CONTINUE
       GO TO 461
 1461 CONTINUE
      THIS SECTION OF THE PROGRAM ANALYZES THE DATA USING THE FAST
С
С
      FOURIER FIT, RHARM.
       M=12
```

```
ISET=0
     CALL RHARM(Y, M, INV, S, IFERR)
      IF(KREP.GE.0) GD TO 1502
1503 READ(1,1556) KREP, FFIRST, FLAST
     WRITE (3,2) (HEAD(I), I=1,10)
1556 FORMAT(12,2E15.5)
1502 CONTINUE
      FACTOR=1./(NPTS*DRH)
      RFR=1./FACTOR
      KFIRST=FFIRST/FACTOR
      KFIRST=(KFIRST*2)+1
      KLAST=FLAST/FACTOR
      KLAST = (KLAST \neq 2) + 1
      WRITE(3,1550) KFIRST, KLAST, RFR
      IF(KLAST-KFIRST-398.GT.0) GO TO 1510
      GO TO 1515
1511 CONTINUE
      J=0
      DO 1500 K=KFIRST,KLAST,2
      J=J+1
      Z(J) = Y(K) * Y(K) + Y(K+1) * Y(K+1)
      W = (K - 1)/2
      UU(J)=W*FACTOR
1500 CONTINUE
      CALL FIT(J,Z,UU,UU1,Z1,RATION,LK)
      IF(MPTS) 1505,1506,1506
15C6 CALL GRAPH(J,UU,Z,KS,4,12.,10.,0,0,0.1,0.,XLAB1,YLAB1,
    1GLAB1,GLAB2)
15C5 CONTINUE
      DO 1507 I=1.LK
        UU2(I) = UU1(I) * RFR
      ZZ(I) = ZI(I)
      Z1(I) = Z1(I)/RATION
15C7 CONTINUE
      WRITE(3,1551) RATION
      WRITE(3,1552)
      WRITE(3,1553) (UU1(I), Z1(I), ZZ(I), UU2(I), I=1, LK)
```

```
KFIRST= ',I6,' KLAST= ',I6,' DELT(1/H)= '
 1550 FORMAT("O
     1,E12.3)
1551 FORMAT("0
                   NORMALIZING FACTOR (FAST FOURIER FIT) = •,E10.3)
1552 FORMAT(*O FAST FOURIER FIT ANALYSIS*/*O FREQUENCY
                                      INTENSITY
             NORM. INTENSITY
                                                       COEFFICIENT ///
    1
 1553 FORMAT(E20.5,E26.5,E19.5,F20.1)
      IF(ISET.GT.0) GO TO 1512
      IF(KREP.LT.0) GO TO 1503
      GO TO 461
 1510 KLASTP=KLAST
      KLAST=KFIRST+398
      WRITE(3,1554)
1554 FORMAT("O THE DATA WILL BE ANALYZED IN SECTIONS")
      ISET=1
 1515 CONTINUE
      FFIRST=((KFIRST-1)/2)*FACTOR
      FLAST=((KLAST-1)/2)*FACTOR
      WRITE(3,601) FFIRST
      WRITE(3,602) FLAST
      GO TO 1511
 1512 KFIRST=KLAST-20
      KLAST=KFIRST+398
      WRITE (3,2) (HEAD(I), I=1,10)
      IF(KLAST-KLASTP.GT.O) GO TO 1520
      GO TO 1515
 1520 KLAST=KLASTP
      ISET=0
      GO TO 1515
  461 CONTINUE
     CALL STOPTM(DELT)
      WRITE (3,699) DELT
  659 FORMAT (62X, TIME USED IN EXECUTION (SEC), F8.2)
 424 CONTINUE
С
     THE FIRST CARD OF THE NEXT DATA SET IS READ. IF THIS CARD IS A BLANK,
     THE PROGRAM ENDS.
С
     READ (1,1) RATE, HSCALE, HZERO, THETA, COILK, TZERO, QQQ, KREP, NADD,
    1(HEAD(I), I=1, 10)
```

```
501 IF (RATE) 5,450,5
  450 IF (COILK) 5,451,5
  451 WRITE (3,452)
                     END DE DATA GUTMAN A331 PHYS 4-3733
                                                            • • •
  452 FORMAT("1
      STOP
      END
С
      SUBROUTINE FIT (NUM,Z,UU,UU1,Z1,RATION,NUM1)
С
      THIS SUBROUTINE FINDS THE PEAKS IN THE SPECTRUM
С
      THE Z.UU.ZI.UUI ARRAYS MUST BE DIMENSIONED IN THE CALLING PGM.
С
С
      NUM1=# OF POINTS RETURNED BY Z1 OR UU1 ARRAYS.
Ç
      NUM=# OF POINTS SUPPLIED IN Z OR UU ARRAYS.
С
      RATION = LARGEST VALUE OF Z OR Z1 ARRAYS.
С
      NZ1MAX=SIZE OF Z1 ARRAY AS DIMENSIONED BY CALLING PGM.
С
           7 = AMPLITUDE OF DATA UU = FREQ OF CORRESPONDING DATA.
С
                                      UU1 = FREQ OF CORRESPONDING PEAKS.
           Z1 = HEIGHT OF PEAKS
С
       .
      DIMENSION Z(200), UU(200), Z1(99), UU1(99)
      DIMENSION X1(3), X2(3), W(3)
      DOUBLE PRECISION A(4)
      NZ1MAX = 99
      Z1(1)=0.0
      K=0
      I=1
      IF (Z(2)-Z(1)) 405,407,401
  407 I=2
 401 IF (Z(I+1)-Z(I)) 403,403,402
 402 I=I+1
      IF (I-NUM) 401,410,410
 405 IF (Z(I+1)-Z(I)) 406,401,401
  406 I = I + 1
      IF (I-NUM) 405,410,410
  403 DO 404 J=1,3
      NM=I+J-2
      W(J) = 1.0
     X1(J)=UU(NM)
```

```
404 X2(J) = Z(NM)
      CALL OPLSPA (2,3,X1,X2,W,A,0.0)
      K = K + 1
      UU1(K) = -A(2)/(2 \cdot A(3))
      Z1(K) = A(1) - (A(2) * A(2)) / (4 * A(3))
      IF (K-NZ1MAX) 405,844,844
  844 WRITE (3,846) NZ1MAX
  845 FORMAT ('O ****** THERE ARE MORE THAN ', I3, PEAKS *******)
  410 NUM1 = K
      IF (NUM1) 430,430,432
  430 WRITE (3,431)
                         THERE ARE NO PEAKS IN THIS DATA SET!)
  431 FORMAT ( 0
      RATION=Z(1)
      IF (Z(NUM) .LE. RATION) GO TO 415
      RATION=Z(NUM)
  415 Z1(1) = RATION
       GO TO 414
  432 CONTINUE
      RATION = Z1(1)
  41.2 DO 413 K = 1.NUM1
      IF (Z1(K) .LE. RATION)
                                   GO TO 413
      RATION = ZI(K)
  413 CONTINUE
С
      THE Z'S ARE NORMALIZED. THE ZI'S WILL BE NORMALIZED IN THE MAIN PROGRAM.
  414 DO 425 I=1.NUM
  425 Z(I) = Z(I) / RATION
    L CONTINUE
      RETURN
      END
С
      SUBROUTINE FILTER (OUT, IMIN, IMAX, XSTEP, UO, QQQ, NCOL, KMAX, OUT2)
С
      QQQ = Q OF SYSTEM
С
      UO = PASS FREQUENCY
С
       XSTEP=DRH, INCREMENT ALONG INVERSE-B AXIS. KMAX=1, BY STEAD1
С
      IMIN = 1 SET BY MAIN. IMAX=NPTS, USUALLY 10000 OR LESS.
      DIMENSION Z(1001)
       COMMON XLAB(5),YLAB(5),Y(8200),INV(2100),S(2100)
```

```
EQUIVALENCE (INV(1),Z(1))
      DOUBLE PRECISION XSTEP
  500 KS=3
      00=0.
      QP=0
      DUT=0.
      -0UT2=0.
      K=IMIN
      M=1
   40 H=UO*XSTEP
      IF (H) 4,4,5
    4 H=−H
    5 CONTINUE
                .
      PARAMETERS ARE SET UP.
С
      A1=1.-H*H/2.
      A2=H*(1.-H/(2.*QQQ))
      A3=H*H/2.
      A4=1.-H/QQQ
      A5=-H
  501 I=1
      L=1
      DO 1 J=1,NCOL
    1 Z(J) = 0.
С
С
      THIS IS THE BASIC PART OF THE FILTER. THE EQUATIONS APPROXIMATE THE
С
      RESPONSE QQ(K) OF A FILTER TO A FORCING FUNCTION Y(K)--THE INPUT DATA.
С
            QQ(K+1) = A1*QQ(K) + A2*QQ'(K) + A3*Y(K)
С
С
            QQ^{(K+1)} = A4*QQ^{(K)} + A5*QQ(K) + H*Y(K)
    5 QQ1=A1*QQ+A2*QP+A3*Y(K)
      QP = A4 * QP + A5 * QQ + H * Y(K)
      00=001
      IF (K-KMAX) 3,15,15
      KMAX=1 BY STEAD1, SO STEP 15 IS NEXT.
С
С
      THE FILTER OUTPUT IS COLLECTED HERE.
                                              OUT21 IS THE SUM OF THE SQUARES
      OF THE AMPLITUDES OF THE RESPONSE.
C
   15 OUT2=OUT2+QQ*QQ
```

```
THE PERIODOGRAM IS SET UP HERE. A RESPONSE AMPLITUDE QQ IS ADDED TO Z(I)
С
С
      EVERY NORL TIMES. IF UO COINCIDES WITH A FREQUENCY CONTAINED IN THE DATA.
С
      7(1) WILL BE SUMMED FOR THE SAME PHASE OF THE CYCLE OF QQ EACH TIME, AND
      THE SUMMATION WILL BE COHERENT.
С
      Z(I) = Z(I) + QQ
      IF (00-30000) 71,71,72
   72 WRITE (3,73) DUT2,QQ,K,Y(K)
   73 FORMAT ( TILT* OUT2=',E14.3, QQ=',E15.4, Y(',I4,')=',E20.4)
      M=M+1
      IF (M-5) 71,71,74
   74 GO TO 9
   71 CONTINUE
      I = I + 1
      IF (I-NCOL) 3,3,2
    2 I=1
      L=L+1
    3 K=K+1
      IF (K-IMAX) 6,9,9
С
      L COUNTS THE NUMBER OF TIMES A QQ AMPLITUDE IS PLACED IN EACH Z(I).
    9 ZSUM=0.
      DO 10 I=1, NCOL
   10 ZSUM=ZSUM+Z(I)/L
      ZSUM=ZSUM/NCOL
C.
      L \neq NCOL = NPTS - ZSUM IS THE AVERAGE PERIODOGRAM RESPONSE Z.
      OUT=0.
С
      THE MEAN SQUARE OF THE PERIODOGRAM RESPONSE IS TAKEN, AND CALLED 'OUT'.
      DO 11 I=1,NCOL
   11 OUT=OUT+(Z(I)-ZSUM) **2
      OUT=OUT/NCOL
      THE FILTER RESPONSE IS 'OUT2'.
С
      OUT2=OUT2/(IMAX-KMAX)
      RETURN
      END
С
      SUBROUTINE BFIELD (H, IMAX, THETA, HO)
      DIMENSION H(1)
      P = (COS(THETA)) * * 2
```

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```
X=H0*(3.*P-1.)/2.
      Y=H0*P
      DO 1 I=1, IMAX
    1 H(I) = HO + H(I) * (H(I) + X) / (H(I) + Y)
      RETURN
      END
С
      SUBROUTINE STEADF(QQQ, MPTS, DRH, H1, THETA, HZERO, HEAD, F1, F2, RES,
     1TIMEM, KMAX, NPTS)
      THIS SUBRDUTINE READS IN THE DHVA DATA Y (DIMENSION OF 4000)
С
С
      AND CALLS STEAD1.
С
      THE SECOND CARD IN THE DATA SET IS READ.
С
      NOPT=1 IF THE FIELD IS READ ONLY AT START AND STOP--USUAL CASE.
      H1 AND H2 REPRESENT THE INITIAL AND FINAL MAGNETIC FIELDS IN MA
С
С
      OR KHZ DEPENDING ON FOPT.
С
      FOPT=0., H1 & H2 ARE IN MILLIAMPS.
С
      FOPT=1., H1 & H2 ARE AL. NMR FREQ. IN KHZ.
С
      FOPT=2., H1 & H2 ARE F. NMR FREQ. IN KHZ.
С
      FOPT=3., H1 IS AL. & H2 IS F. NMR FREQ. IN KHZ.
      FOPT=4., H1 IS F. & H2 IS AL. NMR FREQ. IN KHZ.
С
С
      MPTS IS USED AS A CONTROL ON WHAT WILL BE GRAPHED
С
      NSTRT SPECIFIES FROM WHAT POINT THE HIGH-FIELD INPUT DATA WILL BE USED.
С
      DUP! IS USED TO SAVE THE DATA ON DISC. WHEN THE DATA IS READ IN,
С
      SET 'DUP' = -1. THEN TO RECALL DATA FROM DISC, E.G., TO SCAN A
С
      DIFFERENT FREQUENCY RANGE USING FILTER, SET "DUP" = +1, EACH TIME
С
      DATA IS TO BE RECALLED.
                                 *** NOTE *** THE FIRST AND SECOND CARDS
      OF THE DATA SET MUST BE SUPPLIED EACH TIME THE DATA IS RECALLED
С
      FROM DISC. BE SURE TO INCLUDE A JCL CARD SUPPLYING DEVICE 4 =
С
С
      DISC (SYSDA):
С
    //GD.FT04F001 DD SPACE=(800,(120,15)),DISP=(,DELETE),DSN=&RP,UNIT=SYSDA
С
С
      SCFRI IS A SCALE FACTOR USED TO MAKE CONSTANT AMPLITUDE DATA
С
      BY INCREASING THE AMPLITUDE AT THE LOW FIELD END.
С
      DIMENSION Y(4000), H(4000), JAZZ(30)
      DIMENSION GLAB1(5), GLAB2(5), HEAD(1)
      DOUBLE PRECISION DRH
```

```
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```

```
COMMON XLAB(5), YLAB(5), QQ( 8200), INV(2100), S(2100)
    EQUIVALENCE(INV(1),H(1))
   READ(1,1)NOPT,H1,H2, SCFR,DT1,F0PT,F1,F2,RES,TIMEM,MPTS,NSTRT,DUP
   DELT = 1.0
 1 FORMAT(I2,2F6.0,3F9.3,2E9.2,F6.3,F2.0,I2,I5,4X,F2.0)
   DO 3 I=1,5
   GLAB1(I) = HEAD(I)
 3 GLAB2(I)=HEAD(I+5)
   IF (MPTS) 30,31,32
30 WRITE (3,33)
33 FORMAT (
                 NO GRAPHS PLOTTED!)
   GO TO 42
31 WRITE (3,34)
34 FORMAT (
                 INPUT WAVEFORM AND OUTPUT SPECTRA PLOTTED ()
   GO TO 42
32 WRITE (3,35)
                 ONLY THE OUTPUT SPECTRA GRAPHED")
35 FORMAT (
42 IF(DUP.GT.0.0) GD TO 55
   I = FOPT + 1.
   GD TO (60,61,62,63,64),I
60 GM2=1./3.0469
   GM1=1./3.0469
   GO TO 41
61 GM1=1.11118
   GM2=1.11118
   GO TO 41
62 GM1=4.0055
   GM2=4.0055
   GO TO 41
63 GM1=1.11118
   GM2=4.0055
   GO TO 41
64 GM1=4.0055
   GM2=1.11118
41 CONTINUE
   H1=H1/GM1
   H2=H2/GM2
```

```
11 19=1
      IM=26
   12 READ(1,6) (JAZZ(I), I=1,26)
    6 FORMAT(26A3)
      CALL MESS (JAZZ)
      DO 2 I = 1.26
      KTEMP = IO + I - 1
    2 Y(KTEMP) = JAZZ(I)
      I = IM
      THE CARDS ARE READ ONE AT A TIME. IF THE LAST TWO 3-DIGIT NUMBERS
С
С
      ON THE CARD ARE ZERO, THE DATA SET IS CONSIDERED TO BE TERMINATED.
С
      THEREFORE, IF THE FINAL CARD IN A DATA SET IS FILLED OR HAS ONLY ONE
С
      THREE-DIGIT NUMBER MISSING, AN EXTRA BLANK CARD MUST BE INSERTED
С
      AFTER IT.
      IF (Y(I)) 13,14,13
   13 IO = IO + 26
      IM = IM + 26
      GO TO 12
   14 I=I→1
      IF (Y(I)) 13,16,13
   16 I = I - 1
      IF (Y(I)) 15,16,15
      THE TOTAL NUMBER OF INPUT DATA POINTS IS COUNTED, AND IS CALLED
С
C
      'INPTS'. IT IS DIMENSIONED TO 4000.
   15 INPTS=I
      T=DT1
      DTIME=INPTS
      I = 1
      THE H-ARRAY IS GENERATED, ASSUMING A UNIFORM, LINEAR RAMP FROM
С
C
      H1 TO H2.
   26 H(I) = ((H2-H1)*(T-DT1)/DTIME+H1)
      I = I + 1
      T=T+DELT
      IF (I-INPTS)26,26,170
  170 IINPTS=INPTS
      IF(DUP.EQ.0.0) GO TO 17
       REWIND 4
```

```
WRITE(4) Y.H
       GO TO 17
   55 CONTINUE
       REWIND 4
       READ(4) Y.H
       INPTS=IINPTS
   17 WRITE (3,19) INPTS
   19 FORMAT (64X, "INPTS=", 16)
       IF(SCFR.EQ.0.) GD TO 117
       IF(H(INPTS)-H(1)) 118,118,119
  119 HHI=H(INPTS)
       HLO=H(1)
       GO TO 120
                                                   Υ.
  118 HHI=H(1)
       HLO=H(INPTS)
  120 DO 121 I=1, INPTS
       AMP = ( (SCFR - 1.) * (H(I) - HHI) / (HLO - HHI)) + 1.
  121 Y(I) = AMP \neq Y(I)
  117 CALL STEAD1 (QQQ,MPTS,DRH,H1,THETA,HZERD,Y,H,INPTS,GLAB1,GLAB2,
     1F1,F2,RES,KMAX,NPTS,NSTRT)
      RETURN
      END
С
      SUBROUTINE STEAD1 (QQQ.MPTS,DRH,H1,THETA,HZERO,Y,H,INPTS,GLAB1,
     1GLAB2, F1, F2, RES, KMAX, NPTS, NSTRT)
      THIS SUBROUTINE GENERATES THE EVENLY SPACED ARRAY OF DATA IN 1/B.
С
      DIMENSION X(4000), Y(1), H(1)
      DIMENSION GLAB1(1), GLAB2(1)
       COMMON XLAB(5), YLAB(5), QQ( 8200), INV(2100), S(2100)
      EQUIVALENCE (QQ(1),X(1))
      DOUBLE PRECISION DRH,T
      KS=3
      IF (HZERO) 19,19,18
   18 CALL BFIELD (H, INPTS, THETA, HZERO)
   19 CONTINUE
      IF (NSTRT) 51,51,52
   52 JNPTS = INPTS
```

```
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```

```
INPTS=JNPTS-NSTRT
      IF (H(1)-H(INPTS)) 55,55,56
   56 WRITE (3,57)NSTRT
   57 FORMAT (' COUNT STOPS AT PT', I6)
      GO TO 51
   55 DO 53 I=1, INPTS
       J=I+NSTRT
      Y(I) = Y(J)
   53 H(I)=H(J)
      WRITE (3,58)NSTRT
   58 FORMAT(' COUNT STARTS AT PT', I6)
   51 WRITE (3,54)H(1),H(INPTS),INPTS
   54 FORMAT(
                  FIELD RANGE IS ',2F9.1, 'INPTS=',I6)
      H1 = H(1)
      THE FIELD ARRAY IS INVERTED.
С
      DO 20 I=1, INPTS
   20 H(I) = 1./H(I)
   41 CONTINUE
С
      TO GENERATE 2**M POINTS REQUIRED BY RHARM, USE NPTS=(2**M)-1.
       NPTS = 8191
      DRH IS THE INCREMENT IN 1/B SPACE.
С
   11 DRH=(H(INPTS)-H(1))/NPTS
  675 C12=0.
      DO 27 I=1. INPTS
   27 C12=C12+Y(I)
      W = INPTS
      C12=C12/W
      DO 28 I=1, INPTS
   28 Y(I) = Y(I) - C12
      IF (MPTS) 32,31,32
   31 00 29 I=1, INPTS
      X(I) = I/2.
   29 CONTINUE
      CALL GRAPH(INPTS, X, Y, KS, 4, 12., 10., 0, 0, 0, 0, XLAB, YLAB, GLAB1, GLAB2)
   32 CONTINUE
      K=1
      I=1
```

```
T=H(1)
      HERE THE ACTUAL DATA ARRAY QQ IS GENERATED. THE POINTS QQ(FCTN OF 1/B)
С
      ARE SPACED BY INCREMENTS OF DRH IN 1/B SPACE, AND ARE FOUND BY INTER-
С
С
      POLATING BETWEEN THE TWO NEAREST INPUT DATA POINTS.
                                                              THIS ARRAY
      QQ IS CONNECTED THROUGH COMMON TO THE Y ARRAY IN "FILTER".
C
   21 QQ(K) = (Y(I+1)-Y(I))*(T-H(I))/(H(I+1)-H(I))+Y(I)
      K = K + 1
      T=T+DRH
      IF (DRH) 22,22,24
   22 IF(T-H(I+1)) 23,21,21
   23 I=I+1
      IF (I-INPTS)21,26,26
   24 IF (T-H(I+1)) 21,21,30
   30 I=I+1
      IF (I-INPTS)21,26,26
   26 CONTINUE
      KMAX=1
      THE NUMBER K (=NPTS) OF INTERPOLATED DATA POINTS IS NOTED.
С
      WRITE(3,987) K
      FORMAT(64X, "K=", I10)
987
      IF (DRH) 1,2,2
    1 \text{ DRH} = -\text{DRH}
    2 CONTINUE
      NOW RETURN TO "MAIN".
С
      RETURN
      END
С
      SUBROUTINE MESS (JAZZ)
         THIS ROUTINE TRANSLATES THE FIRST 26 ELEMENTS OF THE ARRAY
С
         JAZZ FROM THREE DIGIT NUMERIC WITH A MINUS PUNCH OVER THE
С
С
         HIGH ORDER DIGIT IF NEGATIVE (THAT WERE READ UNDER AN
С
         A3 FORMAT CODE) INTO NORMAL INTEGERS.
С
      ALSO CHECKS FOR - PUNCH ONLY AS A HIGH ORDER DIGIT.
С
         THIS ROUTINE IS COMPLETELY IBM 360 MACHINE DEPENDENT
       DIMENSION JAZZ(26), Y(1)
      DO 100 I=1,26
      NA=JAZZ(I)
```

F;	$\frac{1}{10} \frac{1}{10} \frac$
21 23	11 (1) - 10 - 10 - 10 - 10 - 10 - 10 - 10 -
•.	IF (NA) 40.30.30
30	L=-1
	GOTO4
40	M=NA/16777216+15
	IF (M) 3,60,60
3	L=-1
	M=M+32
60	N=N*10+M
۷.	NA=NA*256
80	JAZZ(I)=ISIGN(N,L)
100	CONTINUE
	RETURN
	END
//60.1	114FOUI DD SPACE=(800,(120,15)),DISP=(,PASS),DSN=&SM,UNII=SYSDA
//60.3	
στι	E NUMBER AMPLIIUDE – FIELD DHVA FREQUENCY INTENSITY DATA

//S3 EXEC PLOT, PLOTTER=INCRMNTL