Effect of Magnetic Breakdown and Nonlinear Magnetization on the High-Field Magnetoresistance of Be

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(Received 7 November, 1969)

The high-field magnetoresistance of Be exhibits large-amplitude quantum oscillations as a function of magnetic field for the field parallel to the hexagonal axis. A low frequency, which appears only at temperatures below 4.2°K, cannot be related to a Fermi-surface area. It is demonstrated how this frequency is generated through the interaction of magnetic breakdown and the magnetic domains reported by Condon.

I. INTRODUCTION

PREVIOUS galvanomagnetic measurements[1–3] have shown Be to be a compensated metal ($n_e=n_h$) with only closed pieces of Fermi surface. These pieces,[4] shown in Fig. 1, consist of a "coronet" of holes centered on Γ and a "cigar" of electrons centered on K. However, the energy gap between the coronet and the cigar is sufficiently small that magnetic breakdown[5,6] between these two pieces occurs for magnetic fields greater than ~20 kOe. Galvanomagnetic measurements[2] have shown that this breakdown produces $\langle 10\bar{1}0\rangle$-directed open orbits when the field is in a $\{10\bar{1}0\}$ plane and within 19.5° of the [0001] axis. For **H**‖[0001] the breakdown produces only closed orbits which cause a loss of compensation ($n_e \neq n_h$).

Associated with the magnetic breakdown are large amplitude quantum oscillations in the magnetoresistance similar to those observed in Zn and Mg.[5] However, in addition to the frequency which can be related to the extremal cross sectional area labeled No. 1 (Fig. 1) there is an extra frequency which cannot be related to any extremal area on the Fermi surface. It is the purpose of this paper to demonstrate how this extra frequency is generated through the interaction of the magnetic breakdown and the magnetic domains reported by Condon.[7]

[1] W. A. Reed, Bull. Am. Phys. Soc. **9**, 633 (1964).

[2] W. A. Reed, *Proceedings of the Eleventh International Conference on Low-Temperature Physics St. Andrews, Scotland, 1968*, edited by V. F. Allen, D. M. Finlayson, and D. M. McCall (University of St. Andrews Printing Dept., St. Andrews, Scotland, 1969), p. 1160.

[3] N. E. Alekseevskii and V. S. Egorov, Zh. Eksperim. i Teor. Fiz. **45**, 388 (1963) [English transl.: Soviet Phys.—JETP **18**, 268 (1964)]; N. E. Alekseevskii and V. S. Egorov, *ibid.* **55**, 1153 (1968) [English transl.: *ibid.* **28**, 601 (1969)].

[4] Figure 1 was constructed from band-structure calculations by T. L. Loucks and P. H. Cutler, Phys. Rev. **133**, A819 (1964).

[5] For a review of magnetic breakdown see R. W. Stark and L. M. Falicov, in *Progress in Low Temperature Physics*, edited by C. J. Gorter (John Wiley & Sons, Inc., New York, 1967).

[6] In addition to Refs. 1–3, magnetic breakdown in Be has been reported by B. R. Watts, Proc. Roy. Soc. (London) **A282**, 521 (1964); N. E. Alekseevskii and V. S. Egorov, Zh. Eksperim. i Teor. Fiz. Pis'ma V Redaktsiyu **8**, 301 (1968) [English transl.: JETP Letters **8**, 185 (1968)].

[7] J. H. Condon, Phys. Rev. **145**, 526 (1966).

II. EXPERIMENTAL DETAILS

The samples were sparkcut from a single crystal boule which had been float-zone refined from distilled Be by Nuclear Metals, Inc.[8] The dimensions and residual resistance ratios are given in Table I. Current and potential leads were soldered to the samples which were mounted on a rotatable holder.[9] In addition to the potential leads, sample 406-J-1 had a coil wrapped around it such that its magnetization could be measured for the magnetic field parallel to [0001]. During the course of the measurements it was found that dM/dH is so large in Be that the single loop formed by the potential leads was sufficient to measure the magnetization and a special pickup coil was unnecessary.

The resistance was measured by a standard four-probe dc method. The derivative of the magnetization, dM/dH was measured by modulating the field at 13 Hz and using phase-sensitive detection. The zero suppress on the detector was sufficient so that no bucking coil was required. Magnetic fields up to 100 kOe were generated with a superconducting solenoid.

III. MEASUREMENTS

When the current is in the basal plane and **H**‖[0001] the magnetoresistance is a quadratic function of H at low fields ($H \lesssim 10$ kOe), has a maximum at $H \approx 22$ kOe, and saturates at higher fields. Above about 20 kOe large quantum oscillations appear. This field dependence at 4.2°K is shown in Fig. 2 and at 1.39°K in Fig. 3. At 4.2°K there is a dominant high frequency F_1 of 9.5×10^6 G and only a slight modulation of the envelope. At 1.39°K, F_1 remains but in addition there is a second

TABLE I. Dimensions and residual resistance ratios (RRR) of the Be samples.

Sample[a]	RRR	$l\times w\times t$[b] (mm)	d[c] (mm)
461-*C*-1	3370	8×0.13×0.15	0.29
406-*J*-1	1040	10×1.1 ×1.1	4.4

[a] Both samples had $J\parallel[10\bar{1}0]$.
[b] Length × width × thickness.
[c] Distance between resistance probes.

[8] Nuclear Metals, Inc., West Concord, Mass.

[9] G. F. Brennert, W. A. Reed, and E. Fawcett, Rev. Sci. Instr. **36**, 1267 (1965).

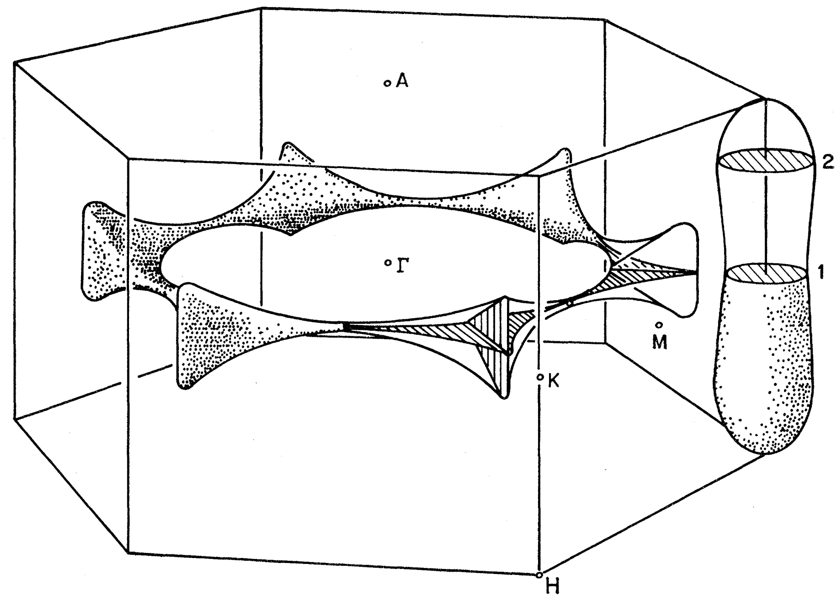


Fig. 1. Fermi surface of Be (see Ref. 4).

frequency of 0.3×10^6 G which is locked in phase with a beat or amplitude modulation of F_1. This low frequency is equal to the difference between F_1 and F_2. F_2 is the frequency associated with the cross sectional area labeled No. 2 in Fig. 1.

In order to investigate the possible relation of the magnetoresistance to the magnetization, sample 406-J-1 was used and both $\Delta\rho/\rho$ and dM/dH were measured simultaneously in the field range 25 to 37 kOe at several temperatures. Figures 4(a)–4(c) show the results of these measurements at 4.2, 2.58, and 1.35°K, respectively. As the temperature is lowered the low frequency and the beats in the high frequency appear simultaneously in $\Delta\rho/\rho$ whereas the dM/dH shows a relatively simple beat pattern at all temperatures.

Closer examination of the data in Fig. 4 reveals that the high frequencies are not identical, there being 33 oscillations in $\Delta\rho/\rho$ for every 34 oscillations in dM/dH. This is due to the fact that the magnetoresistance oscillations are dominated by the magnetic breakdown

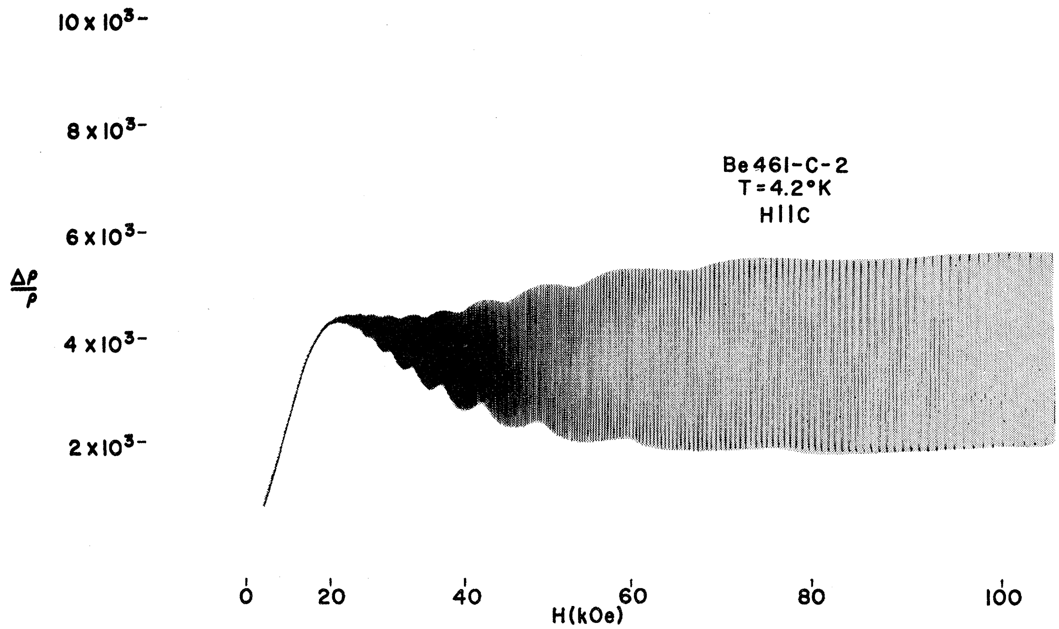


Fig. 2. Field dependence of the magnetoresistance for $H\|[0001]$ at $T=4.2$°K.

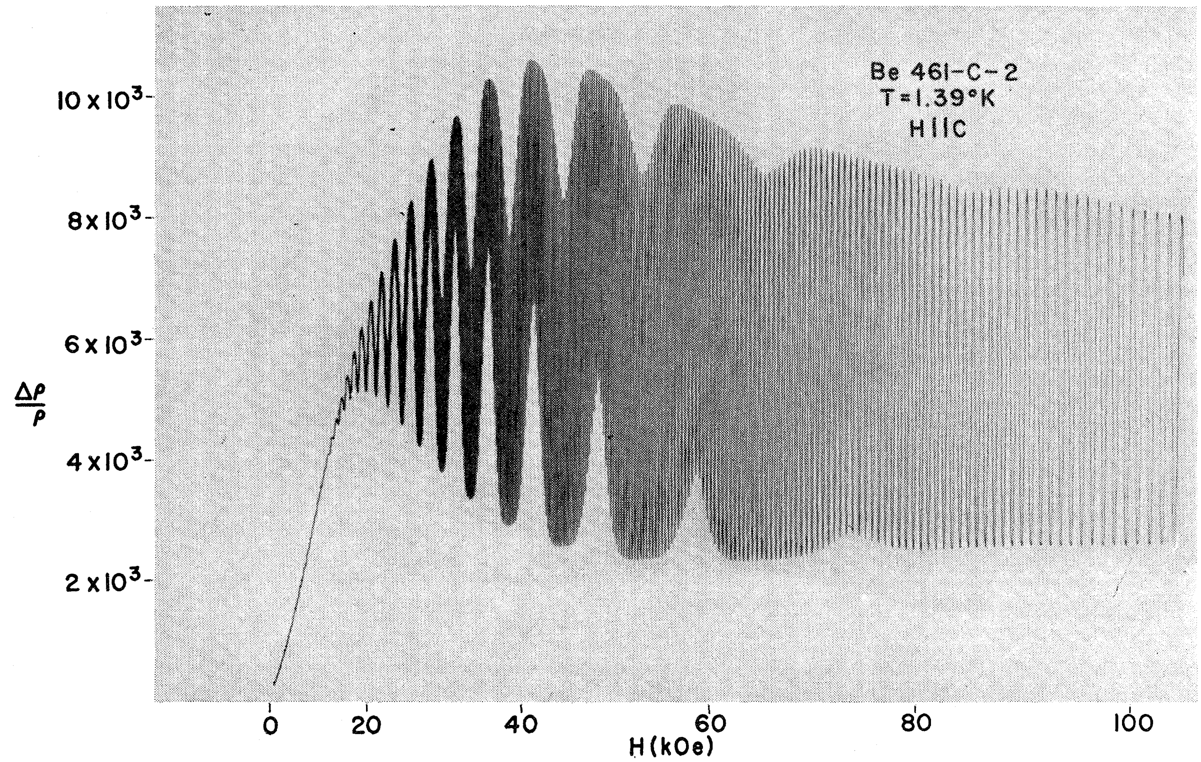


FIG. 3. Field dependence of the magnetoresistance for $H \| [0001]$. Same conditions as in Fig. 2 except $T=1.39$°K.

between the waist orbit (orbit 1 in Fig. 1) and the coronet, whereas the hip orbits (orbit 2 in Fig. 1) contribute twice the magnetization as the waist and thereby dominate the oscillations of dM/dH.

The line shapes of the $\Delta\rho/\rho$ oscillations are not sinusoidal but are rounded at the bottom and pointed at the top at the antinodes of the beats and just the reverse at the nodes. These line shapes are quite different from the line shapes measured in the magnetization.[7]

IV. DISCUSSION

The large amplitude oscillations with frequency F_1, and the change from a quadratic to a saturating field dependence of the monotonic magnetoresistance are well understood in terms of magnetic breakdown between the cigar and the coronet. Similar situations which exist in Zn and Mg have been discussed in detail by Stark and Falicov.[5] However, the difference frequency which appears only at the lower temperatures and is phase-locked to the beats in F_1 cannot be explained simply in terms of magnetic breakdown.

We expect the oscillatory part of the magnetoresistance to be represented by

$$\frac{\Delta\rho}{\rho}=A_1\sin\left(\frac{2\pi F_1}{B}+\phi\right), \tag{1}$$

where A_1 is a slowly varying monotonic function of the magnetic induction, B and ϕ are the difference in phase between $\Delta\rho/\rho$ and M. The magnetic induction, however, is related to the applied field H in the following way:

$$B=H+4\pi(1-L)M \tag{2}$$

and

$$M=A_2\sin\left(\frac{2\pi F_2}{B}\right). \tag{3}$$

Generally M is small, $B\approx H$, and $\Delta\rho/\rho$ has a simple oscillatory behavior. However when M is large and $\partial 4\pi M/\partial B>1$, the magnetic interaction effect becomes important.

Pippard[10] has discussed the effect of magnetic interactions for a rod-shaped sample where the demagnetization factor L is zero. In this case the solution to Eqs. (2) and (3) is shown as curve a in Fig. 5(a). Using a free-energy argument, Pippard pointed out that the induction inside the sample jumps from points 1 to 2 and the values of B in the regions marked ΔB never occur within the sample. Condon[7] has shown that even for the case of $L=1$ (a disk) magnetic interactions still occur. This is because the free energy can be lowered by the formation of magnetic domains which have in them the value of magnetic induction given by the end points marked 1 and 2 in Fig. 5(a). The magnetic induction

[10] A. B. Pippard, Proc. Roy. Soc. (London) **A272**, 192 (1963).

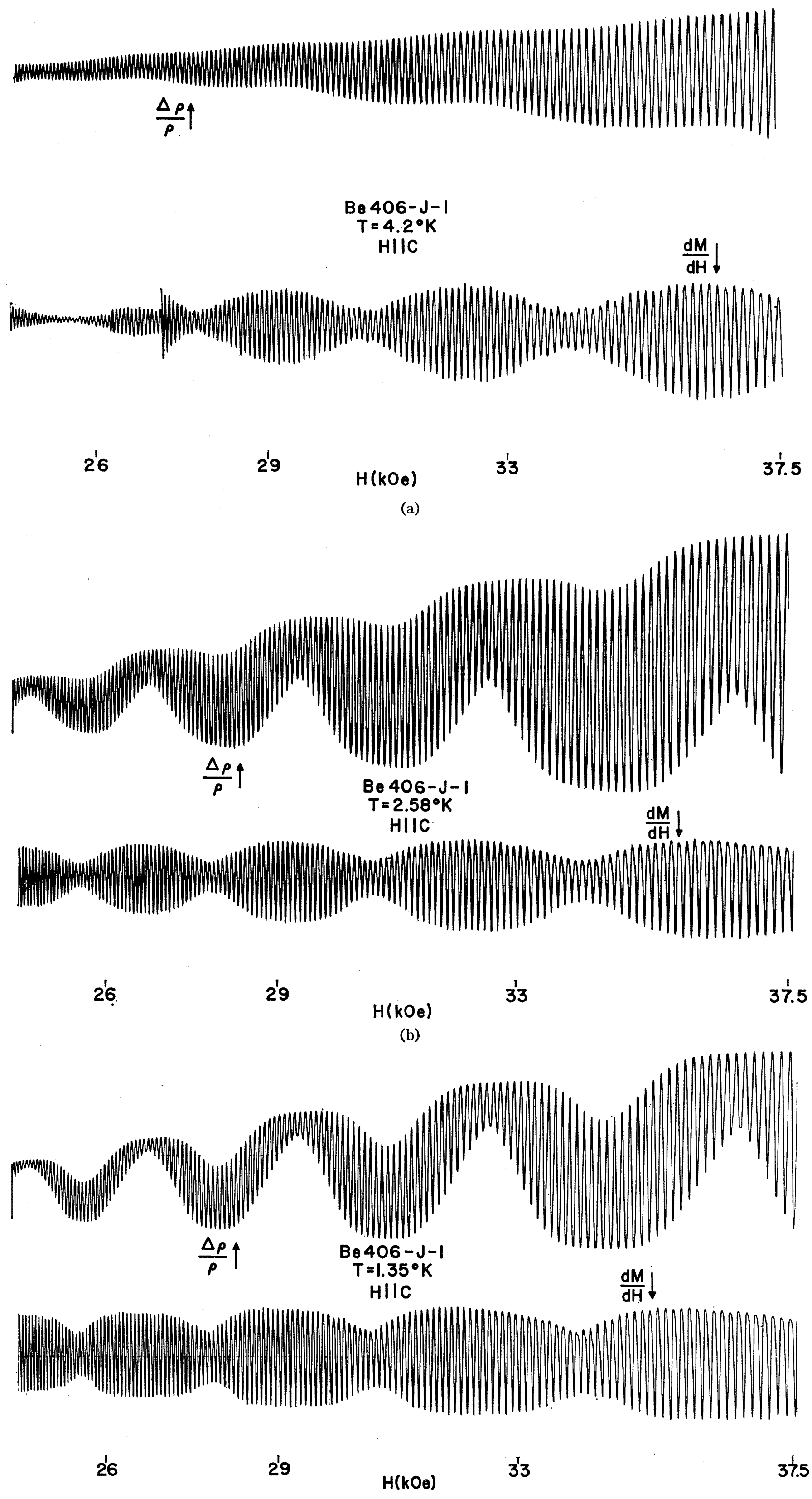


FIG. 4. Field dependence of the magnetoresistance ($\Delta\rho/\rho$) and differential magnetic susceptibility (dM/dH) (a) $T=4.2$°K; (b) $T=2.58$°K; (c) $T=1.35$°K.

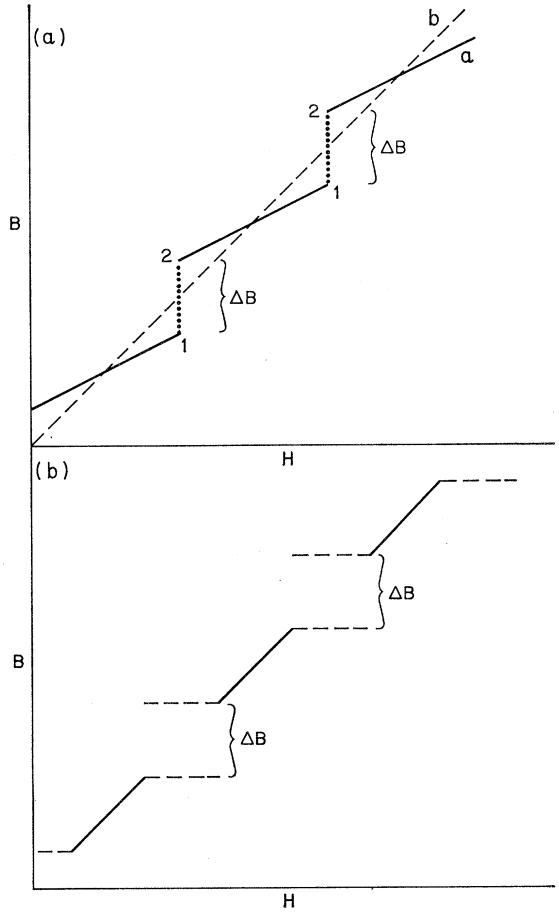


FIG. 5. (a) B versus H, curve a: in regime of magnetic interactions showing discontinuity in B; curve b: $B=H$. (b) B versus H for disk shaped sample ($L=1$). Magnetic domains form in dashed regions of curve.

inside a disk shaped sample[11] is given in Fig. 5(b). The important point is that the same forbidden region ΔB occurs independent of sample shape.

The key to understanding the difference frequency is in the fact that $\Delta\rho/\rho$ oscillates at frequency F_1 whereas the forbidden regions ΔB occur periodically with frequency F_2. The model is then quite simple. When the minima of $\Delta\rho/\rho$ occur in phase with the forbidden ΔB's, these minima are not observed experimentally. Approximately 16 or 17 oscillations of F_1 or F_2 later the phase relation is reserved and the maxima of $\Delta\rho/\rho$ are forbidden. In between these regions the forbidden values of B occur on the sides of the $\Delta\rho/\rho$ oscillations. The net result of these forbidden regions of B is to "carve notches" in the envelope of the magnetoresistance and create the appearance of a low-frequency oscillation which is equal to the difference between F_1 and F_2.

[11] This behavior has been verified by NMR measurements in silver. J. H. Condon and R. E. Walstedt, Phys. Rev. Letters 21, 612 (1968).

The size of ΔB is directly related to the peak-to-peak amplitude of the magnetization. Since the magnetization has a beat with a frequency 0.3×10^6 G, the size of ΔB will oscillate at the same frequency. At the nodes of M the fraction of $\Delta\rho/\rho$ which is lost will be at a minimum and the amplitude of the magnetoresistance oscillations will be at a maximum. At the antinode of M the reverse is true and the amplitude of $\Delta\rho/\rho$ will be a minimum. This then provides an explanation of the amplitude modulation of the magnetoresistance.

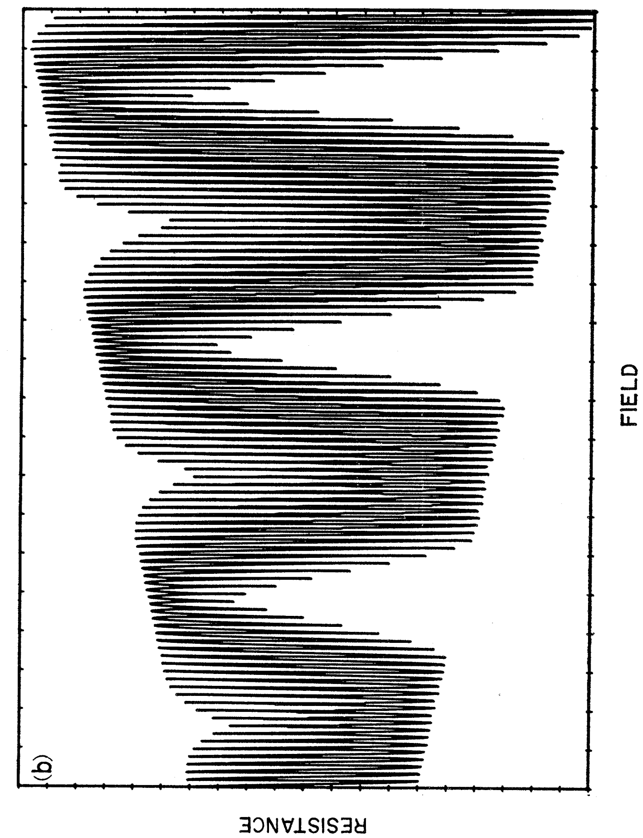
In order to test the validity of the preceding explanations, the physical problem was simulated on a computer. The oscillatory resistance was defined by

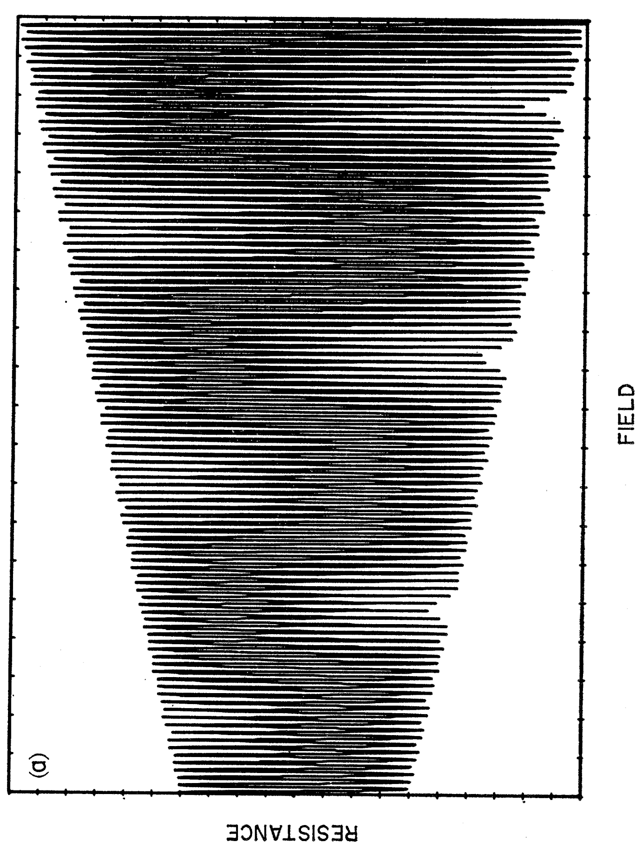
$$\frac{\Delta\rho}{\rho}=C\sin(\omega_1 B+\phi), \tag{4}$$

which over a small range of B is essentially equivalent to Eq. (1). $B(H)$ was defined like curve a in Fig. 5(a). The periodicity of B was taken 3% smaller than the periodicty of the resistance oscillations and the amplitude C was made a linearly increasing function of H. The mean size of ΔB was an adjustable parameter but the instantaneous value of ΔB was made to oscillate about the mean with a frequency of 0.03 $\omega_1/2\pi$ to simulate the effect of the beats in the magnetization. The results of the program are shown in Figs. 6(a)–6(c) for $\Delta B=10$, 30, and 50% of the periodicity of B. These values were chosen so that the results would correspond to the data shown in Figs. 4(a)–4(c). Not only are the primary features of the data reproduced but also the line shapes discussed in Sec. III. The good agreement between the data and the computer output adds credence to the proposed explanations.

The phase relation of the oscillating $\Delta\rho/\rho$ and dM/dH can also be determined from the experimental results. Figure 4 shows that only the maxima of the $\Delta\rho/\rho$ oscillations occur at the antinodes of the dM/dH data. In the region of the antinodes the dM/dH oscillations of frequencies F_1 and F_2 are in phase and, because of the magnetic interactions, only the diamagnetic part of the magnetization is allowed on a microscopic scale.[7] We therefore conclude that the maxima of the magnetoresistance oscillations due to magnetic breakdown occur simultaneously with the minima of the differential susceptibility associated with F_1. Even though this argument does not depend on the reproducibility of the magnetic field between experiments, we have also made the direct comparison of phases and form the same conclusion.

The formation of magnetic domains, or the strength of the magnetic interactions, is dependent upon the ratio of the magnetization to the period of the oscillations in H. At very high fields the amplitude of M is not increasing rapidly whereas the periodicity is still increasing as H^2. This will lead to a decrease in the





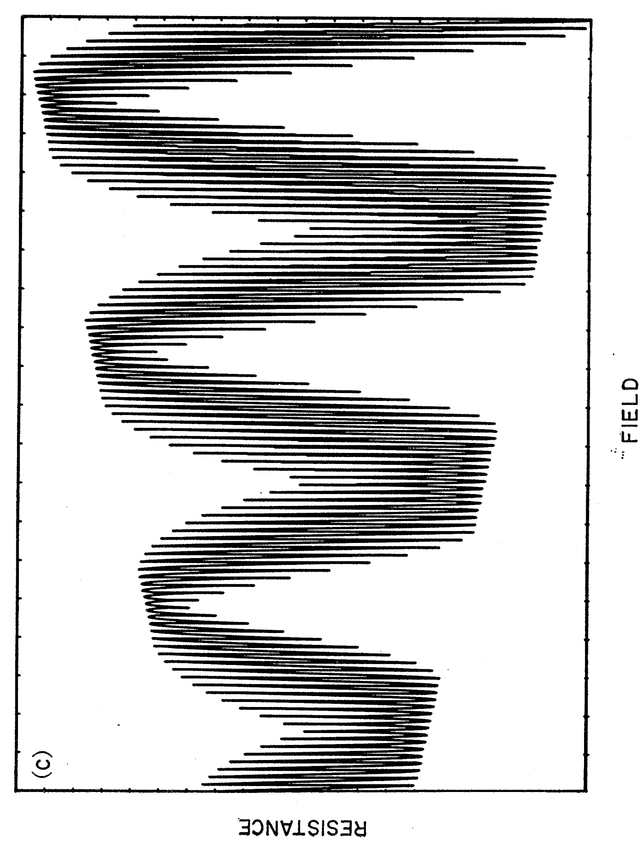


FIG. 6. Computer simulation of magnetoresistance data; (a) $\Delta B = 0.1F_2$, (b) $\Delta B = 0.3F_2$, and (c) $\Delta B = 0.5F_2$.

magnetic interaction effect and a corresponding disappearance of the difference frequency at very high fields. This corresponds to the results shown in Fig. 3.

ACKNOWLEDGMENT

We wish to thank G. F. Brennert for technical assistance.

PHYSICAL REVIEW B VOLUME 1, NUMBER 8 15 APRIL 1970

Non-Central-Force Model of LiH: Phonon Dispersion Curves and He Migration

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(Received 8 December 1969)

Two models for calculating defect properties of LiH (^{7}LiD) are obtained using noncentral interionic potentials of the form $f(\theta,\varphi)\phi(r)$, where $f(\theta,\varphi)$ has cubic symmetry and $\phi(r)$ is a Born-Mayer repulsion taken from quantum-mechanical calculations. The parameters of the models were varied to give the best fit to the interionic spacing, the binding energy, and the elastic coefficients of LiH. Phonon dispersion curves, which can be obtained from only one of the models, are compared with experimental results. Calculations with the two models give 0.69 and 0.87 eV for the activation energy for migration of an interstitial He atom in LiH.

I. INTRODUCTION

In order to calculate the theoretical values of such properties of point defects in solids as local strains and migration energies, it is necessary to have a "model" for the crystal lattice. Recently, several models of the LiH(^{7}LiD) crystal have appeared in the literature. Verble, Warren, and Yarnell[1] have measured the phonon dispersion curves of LiH (^{7}LiD) using neutron diffraction techniques and were able to obtain a satisfactory fit to their data with a seven-parameter shell model. Jaswal and Hardy[2] have applied the distortion-dipole model, including angle-bending forces, to the calculation of the phonon dispersion curves and frequency distribution of LiH (^{7}LiD). They made use of the measured phonon dispersion curves of Verble, Warren, and Yarnell,[1] the interionic distance r_0, the infrared dispersion frequency,[3,4] and the Szigeti effective charge[5] to determine the parameters in their model. Subhadra and Sirdeshmukh[6] were unable to obtain a reasonable model of LiH using central forces alone and concluded that the measured values of the compressibility of LiH are in error. They assigned an upper limit of 2.15×10^{-12} cm^2/dyn to the compressibility. In none of these calculations was the interionic distance determined, i.e., it was always fitted by adjusting the parameters in the various models. Recent calculations of the repulsive interactions between the constituents of LiH by Fischer *et al.*[7] give these interactions as a function of the H^- screening parameter δ. Thus the interionic distance, binding energy, and compressibility can now be determined for various values of δ. Using these central forces determined from first principles, it was found impossible to fit satisfactorily the crystal data. As in the Subhadra-Sirdeshmukh calculations, the compressibility was always too low when the interionic distance and binding energy were within reasonable limits.

The purpose of the present work is to obtain a model of LiH (^{7}LiD) which gives a reasonable fit to the experimental values of interionic distance, binding energy, and elastic constants, and which can then be used to calculate the activation energy for diffusion of a He atom in LiH. Actually, two models were developed—the first gives a reasonable fit to all the experimental quantities mentioned above, but because of a few percent error in r_0 it cannot be used to predict phonon dispersion curves (the Kellerman[8] formalism requires the crystal to be in equilibrium at r_0 and therefore even a few percent error in r_0 invalidates the method). A second model which includes first-nearest neighbors only was fit to r_0 (but fits other experimental quantities less accurately than model I) and used to predict the dispersion curves.

The potentials for the two models are developed in Sec. II, and the phonon dispersion curves predicted by

[1] J. L. Verble, J. L. Warren, and J. L. Yarnell, Phys. Rev. **168**, 980 (1968).
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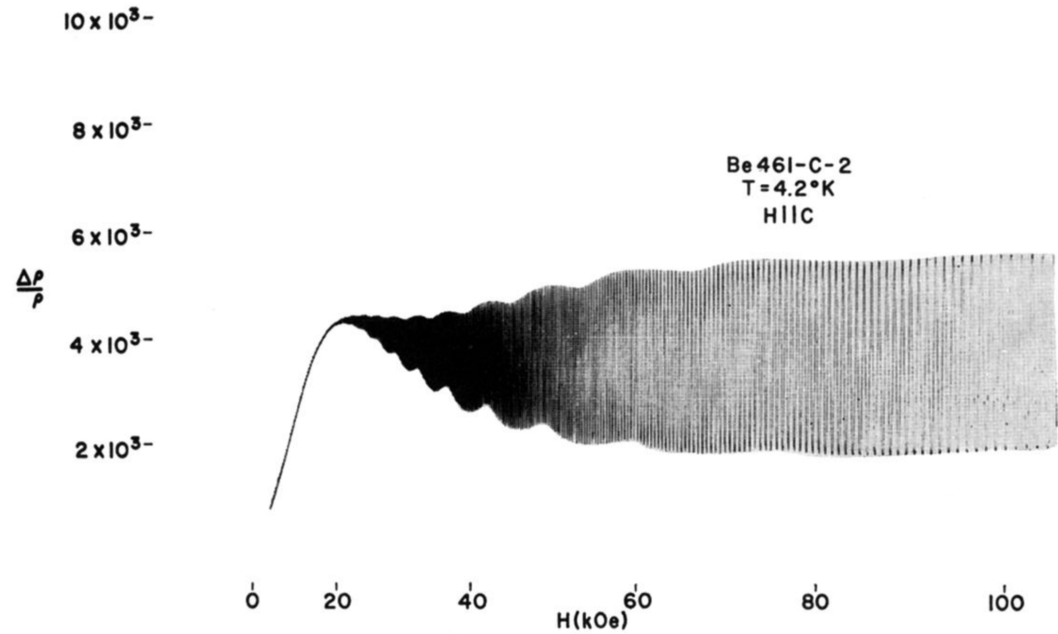


Fig. 2. Field dependence of the magnetoresistance for $H\|[0001]$ at $T=4.2°K$.

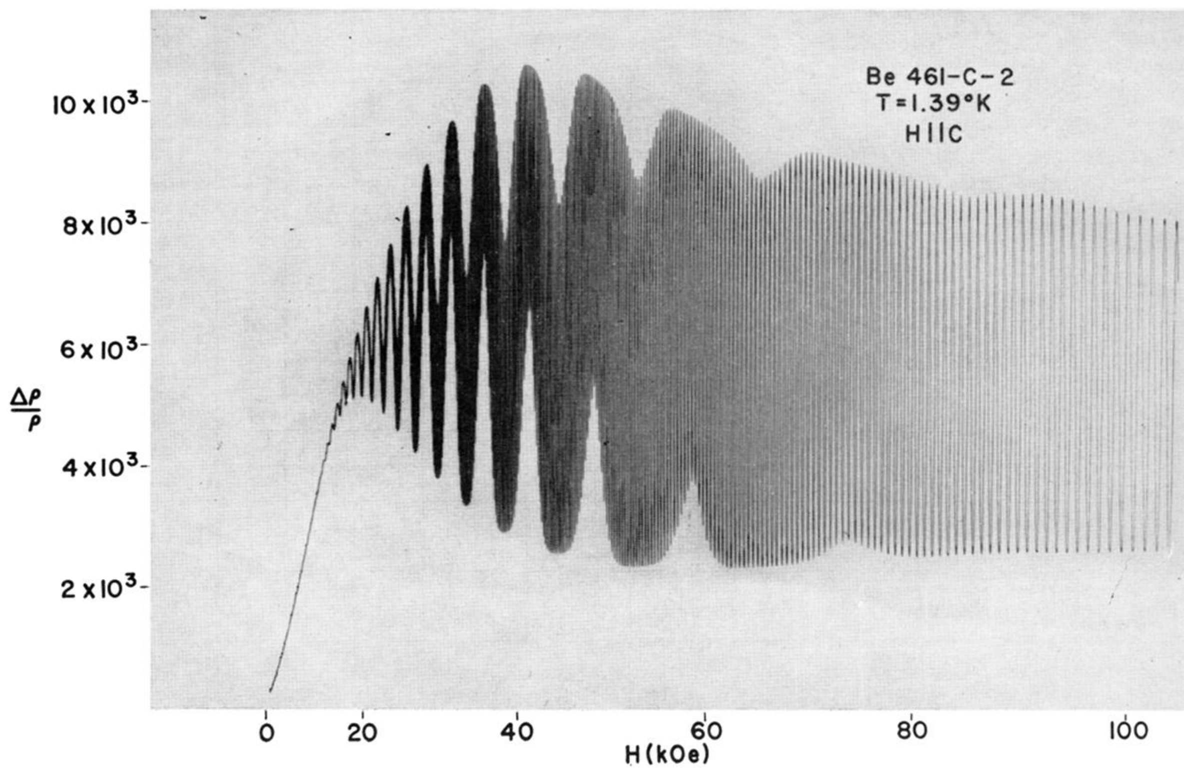
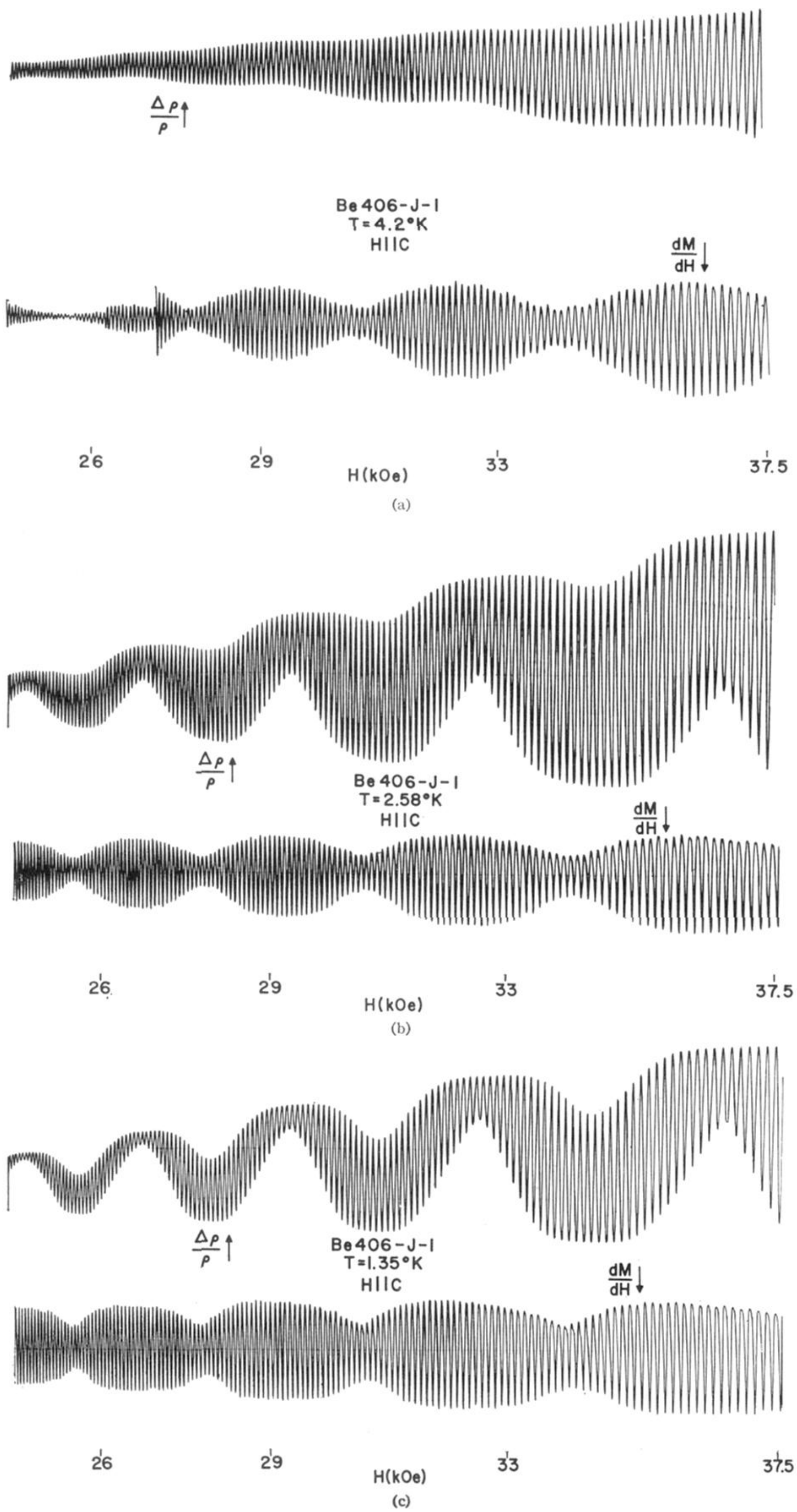


FIG. 3. Field dependence of the magnetoresistance for $H\|[0001]$. Same conditions as in Fig. 2 except $T=1.39°K$.



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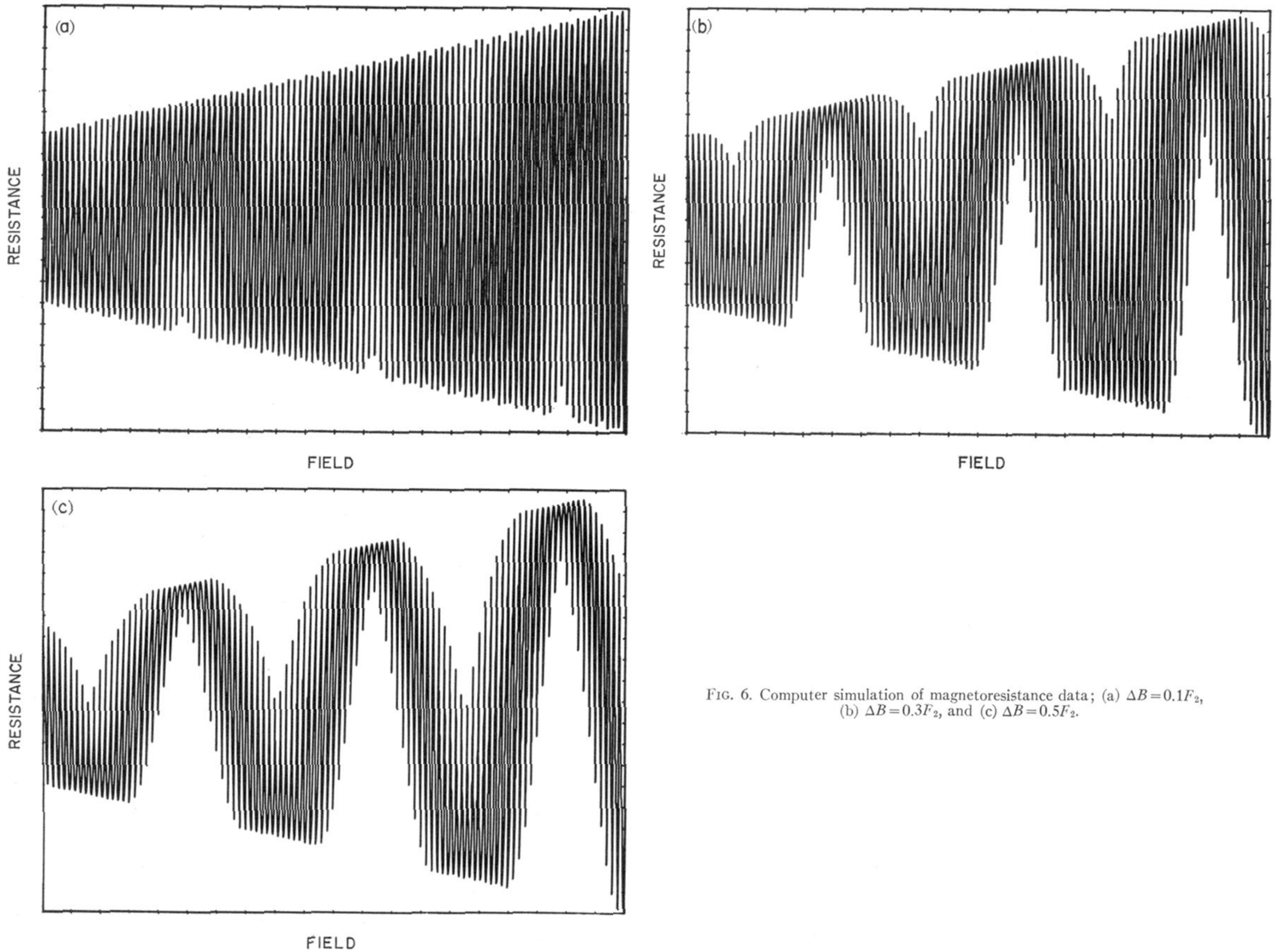

FIG. 6. Computer simulation of magnetoresistance data; (a) $\Delta B = 0.1F_2$, (b) $\Delta B = 0.3F_2$, and (c) $\Delta B = 0.5F_2$.