北海道大学工学部研究報告
第 162 号 (平成 4 年)

Bulletin of the Faculty of Engineering
Hokkaido University, No. 162 (1992)

Anisotropic Cyclotron Effective Mass and Local Fermi Surface Shape of lead

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(Received September 18, 1992)

Abstract

The angular dependence of the Azbel'-Kaner Cyclotron Resonance Peaks in lead is Analyzed. All of the anisotropies in the cyclotron resonance peaks originating from the ⟨110⟩ arms of the Fermi surface in the third band are shown to be characterized by a set of the three effective masses with one negative, corresponding to the hyperboloidal shape of the Fermi surface. This indicates the existence of the hole-electron mixed Landau state adjacent to the extremal points on the Fermi surface where the density of state becomes large. Referring to the 2-D limit of the cyclotron motion in a crystal, we discuss the dynamics of electrons on a hyperboloidal Fermi surface of Pb.

1. Introduction

Investigating the Fermi Surface (FS) for conductive crystals is of particular importance in studies of galvanomagnetic properties, especially, for those oscillatory phenomena with respect to an external magnetic field such as de Hass-van Alphen (dHvA) effect, magnetoresistance and cyclotron resonance (CR), etc. Recent dHvA studies in high T_c superconductors [1,2] or organic superconductors [3,4] have re-shed on the Fermiology. The cyclotron (effective) mass and its anisotropy in connection with the Fermi surface area have customarily been defined by

$$m_c = \hbar/(2\pi)[\partial A/\partial E]_z \qquad (1)$$

where $\hbar$ is the Plank constant devided by (2π) and $[\partial A/\partial E]_z$ is a derivative factor of the extremal Fermi surface area, A, with respect to the energy E. Eq. (1) is however thought to be troublesome when we have to deal with the anisotropic cyclotron mass in conductive crystals whose FS is not known completely, let alone the determination or mapping of the FS from m_c measurements. Although the band calculation has been remarkably successful with respect to geometrical features of the FS of polyvalent metals, it is not so successful with respect to effective masses as determined by cyclotron resonance which measures direct and detailed information of FS, such a way that the method picks out limited groups of carriers on extremal orbits. We shall present in this letter a simple method to treat the anisotropic effective mass in accordance with the Fermiology, report a finding of hyperboloidal FSs

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found in lead and give a discussion over the dynamics of the electron state.

In 1964, M. S. Khaikin and R. T. Mina (KM) [5] first examined the ⟨110⟩ cylindrical arm-like Fermi surface in lead in terms of Azbel' -Kaner cyclotron resonance (AKCR). They reported that the angular dependence of the cyclotron effective mass indicats that the cross-section vertical to the arm axis is not completely circular and the arm itself is in non-cylindrical shape. In 1977, Onuki, Suematsu and Tanuma (OST)[6] also carried out extensive experimental studies on AKCR in lead single crystals, and analyzed the anisotropy of a selection of CR peaks in terms of the corrugated cylindrical ⟨110⟩ arms in the Fermi surface. What is the closed orbit in real lattice space corresponding to the z-orbit around the ⟨110⟩ cylinder in k-space? Why must the corrugated cylinder in k-space be introduced instead of a perfect cylinder? We shall focus on answering these questions by applying our theory on the anisotropy in CR peaks to the case of lead.

If the magnetic field **B** points in the direction μ with respect to the Cartesian coordinate system (x, y, z) (x_1, x_2, x_3) fixed with the crystal, where the x_1 (x_2)-axes in the cyclotronic plane {110} points in the ⟨001⟩ (⟨1$\bar{1}$0⟩) direction, the cyclotron effective mass can be described by

$$m_c=\{\prod_j m_j/\sum_j m_j \cos^2(\mu, X_j)\}^{1/2} \tag{2}$$

where cos (μ, X_j) is direction cosine of a magnetic field in μ direction relative to the orthogonal axes, X_j, fixed in the crystal and m_j's are the masses in the axis direction. It can be shown that all of the angular dependent CR peaks associated with the ⟨110⟩ arms are accounted for the choice of the intrinsic masses, for the best overall fits, $(m_2, m_2, m_3)=(0.94, 0.29, -3.61)m$ for the data by KM and (1.18, 0.244, -8.71)m for those by OST, where m is free electron mass.

2. Anisotropic Cyclotron Effective Mass and Direction Cosine Factor

Consider first the cyclotron motion in a crystalline system under a magnetic field, **B**. A charged particle with charge q in the crystal probably obeys at low temperature equations of motion,

$$m_j\, dv_j/dt=q(\mathbf{v}\times\mathbf{B})_j \quad j=1, 2, 3. \tag{3}$$

Introducing $v_j(t)\equiv\exp(i\omega t)\, v_j$ in (3) we can obtain formula (2) from the secular equation in a straightforward manner [7].

In order to obtain the angle dependence of the CR peaks through formula (2) we must compute the direction cosines explicitly. Assume that the field B is rotated in a plane (pqr) and the rotation angle $\theta$is measured from the initial chosen direction [uvw]. If the coordinate axis direction is further denoted by [hkl], e. g. in X_3 direction, by the law of cosine, we obtain

$$\cos(\mu, X_j)=(hu+kv+lw)/\{(h^2+k^2+l^2)(u^2+v^2+w^2)\}^{1/2}\cos\theta+ \{h(vr-wq)+k(wp-ur)+l(uq-vp)\}/\{(h^2+k^2+l^2)(u^2+v^2+w^2)(p^2+q^2+r^2)\}^{1/2}\sin\theta \tag{4}$$

where X_j = [hkl], the initial field direction, [uvw], and a field **B** is in a plane (pqr) [Azbel'-Kanar CR condition [8]], i.e., **B** is always perpendicular to [pqr].

3. Anisotropic CR Peaks Originating From Pb⟨110⟩ Arm

Using (2) with (4), and choosing the set of effective masses $(m_2, m_2, m_3) = (0.94, 0.29, -3.61)m$ in the three axis directions : [001], [1$\bar{1}$0] and [110], respectively, we obtained the theoretical solid curves in Fig.1 for KM's data of AKCR measurements on Pb⟨110⟩ arm. MK measured [5] CR peaks originating from one of ⟨110⟩ arms by changing the sample plane in which the field was rotate: (1$\bar{1}$0) and (001). As seen in Fig.1, the theoretical agreement with their result (dots) is quite well. In the analysis on AKCR peaks with data by OST[2], we obtained the same tendency of masses but different value $(m_1, m_2, m_3) = (1.18, 0.244, -8.71)m$. Although unclear yet, this difference is possibly due to the difference in the experimental conditions. Since the mass parameter of m_3 is negative the CR peaks shifted upper region of the $(1/\cos\theta)$ line, the dashed -straight- line, in Fig.1. As the extreme condition, if $|m_3| \to \infty$, the CR peaks would appear on the dashed $-1/\cos\theta$ - line. Now that $m_1 \neq m_2$ in this case, m_c showed different angle dependency in a different choice of field rotation planes, (pqr)'s. On the contrary, if $m_1 = m_2$, the CR peaks depend only on the angle from X_3 axes and thus the two solid lines in Fig.1 would degenerate to one line. However from Fig. 1 we can clearly see that the anisotropic CR data indicate $m_1 \neq m_2$ and $m_3 < 0$. The condition of the

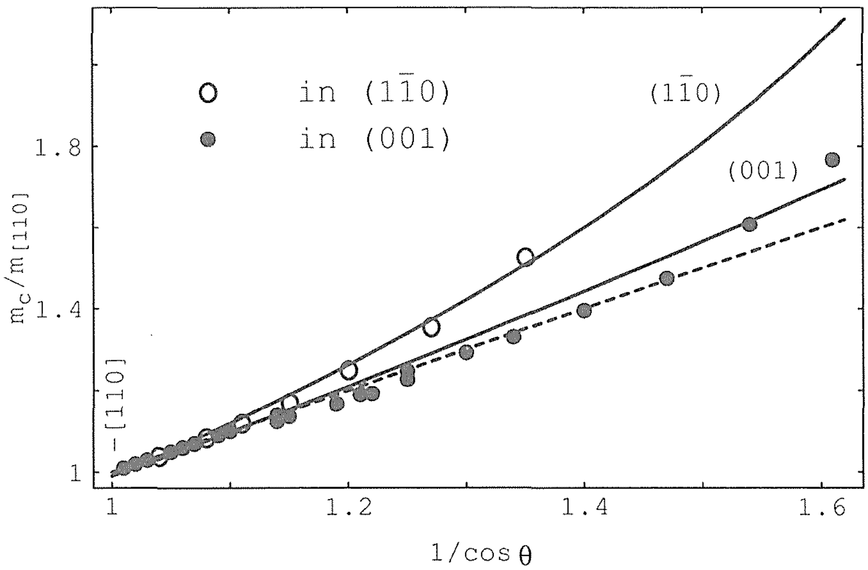

Fig. 1. Anisotropic cyclotron effective mass of the extremal orbital on Pb ⟨110⟩ arm when the field is rotated from [110] in (1$\bar{1}$0) or (001) : $m_{[110]}$ is the cyclotron mass of the field being in [110]. The solid lines are by the present theory with the set of mass (0.94, 0.29, -3.61)m and the dashed line, by the assumption of a cylindrical Fermi surface, while dots are data by Khaikin and Mina (Ref. [5]).

infinit m_3 is the two -dimensional (2-D) limit, i.e. the cyclotron motion of an electron is confined in a plane perpendicular to the X_1-X_2 plane. The cyclotron mass is then reduced to the secant (inverse of cosine) form,

$$m_c = m_0/\cos\theta \tag{5}$$

where m_0 is a geometrical mean of m_1 and m_2, $(m_1 m_2)^{1/2}$, and $\theta$is the angle between the magnetic field and X_3 axis. The 2-D limit is nothing but the condition for a cylindrical FS : The dashed lines in the Fig. 1.

4. Fermi Surface Shape of ⟨110⟩ Arm in Pb

In the present theory we assume three effective masses (m_1, m_2, m_3) for the three direction. These local principal effective masses may be defined on each point of the Fermi surface at the energy $E=E_F$ as the inverses of the principal curvatures given by

$$m_j = \hbar^{-2}[d^2E/dk_j^{\,2}]_{E=E_F} \tag{6}$$

where k_j are the j-components of the k-vector along the principal axes. These local masses defined point-wise, however, cannot be probed readily by experiments. Nonetheless, they are useful concepts. When CR experiments are performed at low temperature, the resonance maxima must be both strong and sharp. Strongly signaled CR peaks are most likely to come from "bellies", "necks" and "caps" of the Fermi surface (see Fig. 2), where the cross-sections perpendicular to the magnetic field are at extrema, therefore the density of state becomes large. Exactly at the same places, the quadratic energy - momentum relations (effective band mass approximations) :

$$E = \hbar^2 k_1^{\,2}/(2m_1) + \hbar^2 k_2^{\,2}(2m_2) + \hbar^2 k_3^{\,2}/(2m_3) \tag{7}$$

are likely to be hold to a great extent than anywhere else. As we shall show in the present work, the CR peaks coming from the Fermi surface of quadratic energy are line-sharp if the electron-phonon interaction and the lattice imperfections are neglected. This means that by analyzing the orientation-dependent CR peaks observed, one can determine the local Fermi surface near "bellies", "necks" or "caps", which are characterized by three principal masses through (2). Note that three (at most) principal masses are needed to characterize the ideally shaped Fermi surface while the two principal masses are sufficient to describe the curvatures at each point of the surface. The actual Fermi surface represented by eq. (7) are ellipsoidal or hyperboloidal depending on the signs of m_j.

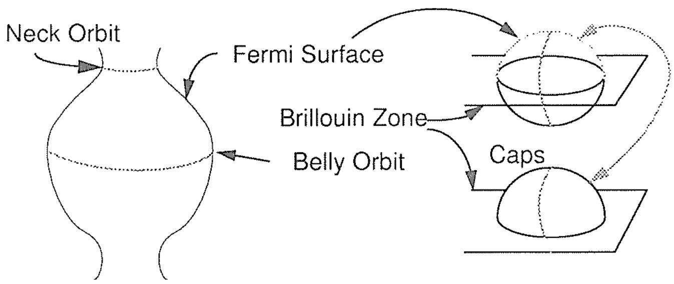

Fig. 2 Neck, belly and cap parts of Fermi surafce.

Let us now examine the Fermi surface of the Pb ⟨110⟩ cylindrical arm. In the present work, we found that the mass of $(m_1, m_2, m_3)=(0.94, 0.29, -3.61)m$ in ⟨001⟩, ⟨1$\bar{1}$0⟩ and ⟨110⟩ direction, respectively. Through this result and (7) with constant $E=E_F$, we can locally predict the Fermi surface shape of the Pb⟨110⟩ arm as schematically illustrated in Fig. 3. The shape is hyperboloidal. Furthermore the cross-section perpendicular to the z-direction, ⟨110⟩, is an ellipse whose semi-axis ratio is given by

$$k_{\langle 001\rangle}/k_{\langle 1\bar{1}0\rangle}=(m_{\langle 001\rangle}/m_{\langle 1\bar{1}0\rangle})^{1/2}=1.80 \quad (8)$$

In the plane contain z-axis, the cross section with the Fermi surface is hyperboloidal because m_3 is a negative mass while the other two are positive. The asymptote is 27°(16°) from the hyperboloid axis direction, ⟨110⟩, in k_1-k_3 (k_2-k_3) plane. The entire third band Fermi surface for the electron in Pb is constructed by all of the six ⟨110⟩ hyperboloidal Fermi surfaces.

Among the models exist in literature for Fermi surface of Pb are of Harrison [9] and van Dyke [10]. The former is known as the nearly free electron model and the latter is a modified model of that of Anderson and Gold [11]. Both models, however, predict the cylindrical shape for the Pb ⟨110⟩ arm with the triangular or the circular cross section. Our model should be differentiated from theirs in the following two points : (1) The cross section of the ⟨110⟩ arm is elliptic -not circular or triangular and (2) the arm is hyperboloidal -not cylindrical.

Little have seemingly been known on the hyperboloidal Fermi surface. In his paper in 1952, however, L. Onsager [12] first inferred the existence of the Hyperboloidal Fermi surface with consideration of the negative curvature of the Fermi surface. Through analysis of the AKCR and anisotropy of cyclotron effective mass in Pb we have had an evidence of its existence.

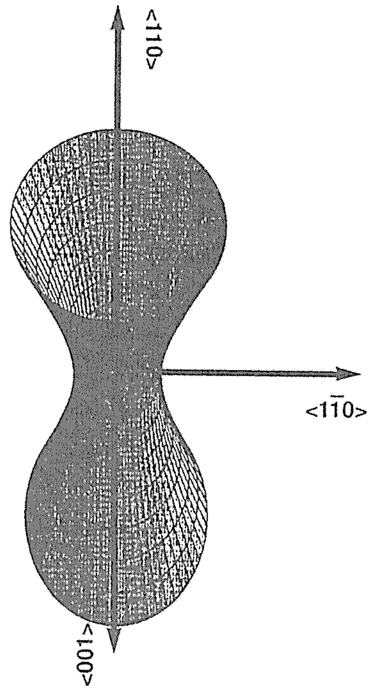

Fig. 3 The local Fermi surface of Pb ⟨110⟩ arm is Hyperboloidal. The cross section perpendicular to the axis, ⟨110⟩ in the figure, is elliptic.

We shall briefly discuss the motion of the Bloch-Landau electron on a hyperboloidal Fermi surface. Consider the case that the magnetic field is applied along the major axis, normal to x_1-x_2 plane. With the positive pair of masses, (m_1, m_2), an electron with negative charge moves around the field counterclockwise. If the number of spiraling electrons per volume is very small, the electrons can be viewed as axially moving with a normal positive mass m_3. This is the case for electrons on ellipsoidal energy surface in Ge and Si [13] for which all of the electron effective masses are found to have the same sign. On the other hand, if the Bloch-Landau electrons within a band are so numerous as to fill up nearly all of the states (orbits), the axial-electron motion is hole-like, i. e. that is characterized by a negative effective mass, m_3. In this case, we may picture that almost all of the "cyclotronic planes", the family of planes parallel to (x_1-x_2), are filled with electrons in accordance with the Pauli principle and a few "vacant" move axially as if they had a positive charge.

5. Conclusion Remarks

In the present work, we have examined the angular dependence of the CR peaks associated with ⟨110⟩ arms of the Fermi surface in Pb. The set of masses obtained for this CR peaks was $(m_1, m_2, m_3)=(0.94, 0.29, -3.61)m$ in KM's data and $(1.18, 0.244, -8.71)m$ in OST's. The Fermi surface corresponding this CR peaks are concluded to be hyperboloidal having elliptic cross-section. Both the present analysis for the KM's data and for OST's data made us confident in the possibility of Pb ⟨110⟩ arm being hyperboloidal. The cyclotron motion of Bloch-Landau electrons is clarified so that they move as if it were a hole in parallel to the hyperboloidal axis while an electron in the perpendicular plane to the axis.

Although almost few reports are exist in literature [14], the hyperboloidal Fermi surface is expected to be seen in the other metals. Such examples of candidates are "neck" part of Cu [15] or other noble metals: the arm of "monster" in hcp metal like Zn or Cd [16]. Like in Pb those parts of Fermi surface in above metals are known to have the open direction. The analyses of the anisotropy in CR peaks, in de Hass-van Alphen effect, in magnetoresistance and in other anisotropic magnetic oscillation phenomena in those metals are now further interest.

We wish to thank Prof. S. Onuki, Dr. H. Kinoshita at Hokkaido Univ. and Prof. S. Fujita at SUNY/Buffalo for several stimulating discussions and suggestions.

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