of the intensities I_+ and I_- of the (210) reflection and I(100) as a function of temperature for the crystal cooled in a 20-oe field. The (100) reflection shows the disappearance of long-range order at $T_N = 66.2 \pm 0.5°$K and the persistence of some short-range magnetic scattering above this temperature. An analysis of the observed polarization ratio, making use of the experimental sublattice magnetization, indicates that the domain distribution remains essentially constant from 4.2°K up to within a few degrees of the Néel point. The details of the domain behavior at temperatures immediately below the Néel point are difficult to establish with precision because of the large changes in the sublattice magnetization occurring within this temperature region and the uncertainty in estimating the proper extinction corrections. However, the observation of $R \neq 1$ up to the Néel temperature suggests that a one-to-one proportion of antiferromagnetic domains is not reached up to the point at which the long-range ordering of the manganese spins disappears.

An unusual feature of the results was the presence of large primary extinction effects, of the type discussed by Hamilton.[4] The size of these effects could be correlated with the degree to which a particular region of the crystal was single domain. It therefore appears that it is the local perfection of the crystal, i.e., the size of the mosaic blocks, that establishes the size of the antiferromagnetic domains.

A second crystal, grown by J. W. Nielsen of the Bell Telephone Laboratories, yielded results which were in every way similar to those obtained from the first crystal, except that the domains were distributed more uniformly in this case.

We gratefully acknowledge the provision of the single-crystal samples by Professor Stout and Dr. S. C. Abrahams.

[1]P. S. Pershan, Phys. Rev. Letters 7, 280 (1961).
[2]Y. Y. Li, Phys. Rev. 101, 1450 (1956).
[3]A. S. Borovik-Romanov, J. Exptl. Theoret. Phys. (U.S.S.R.) 38, 1088 (1960)[translation: Soviet Phys.-JETP 11, 786 (1960)].
[4]W. C. Hamilton, Acta Cryst. 11, 585 (1958).

FERMI SURFACE OF ALLOYS

Hiroshi Sato and Robert S. Toth
Scientific Laboratory, Ford Motor Company, Dearborn, Michigan
(Received February 12, 1962)

The Fermi surface of some metals has been extensively investigated experimentally and its shape has been rather definitely established.[1] In the case of noble metals (Cu, Ag, Au), all the data clearly indicate that the Fermi surface of these metals is not a simple sphere but that it bulges out in the [111] direction and touches the {111} boundaries of the first Brillouin zone. However, in the case of alloys, the situation is not very clear. In the first place, we lack a definite theoretical knowledge of what we mean by the Fermi surface of an alloy although we would expect in general that a Fermi surface similar to that of a pure metal should exist. At the same time, the direct experimental measurement of the Fermi surface of alloys is yet unpractical, because the experimental techniques of these measurements usually require samples with a long mean free path of electrons which can only be attained in highly pure metals.

There is still a series of experimental methods or facts such as the measurement of ordinary transport properties, optical properties, electronic specific heat, etc., which indirectly indicate the shape of the Fermi surface of alloys. However, the interpretation is not yet consistent. Among these, the interpretation of the Hume-Rothery rules based on the Brillouin zone structures is interesting. As is well known, there is too much regularity in the electron-atom ratio at which a definite phase boundary appears in different alloys, for the empirical Hume-Rothery rule to be written off as a mere coincidence. However, the original interpretation of Jones[2] in terms of a spherical Fermi surface has lost its ground with our present knowledge about the shape of the Fermi surface. Some theoretical attempts appeared in order to reconcile this difficulty. For example, Cohen and Heine[3] suggested, particularly for Cu alloys, that the band gap

should decrease significantly and that this would cause the Fermi surface to become spherical upon alloying. On the other hand, Hume-Rothery and Roaf[4] suggested that it was the Fermi surface touching the {200} faces of the Brillouin zone, instead of the {111} faces, that was relevant to the α-phase boundary, and calculated, using the rigid-band model, the electron-atom ratio which gave the phase boundary. Even in such a case there is also the same difficulty as in pure noble metals in reconciling the large distortions of the Fermi surface, in order to allow a reasonable value for the electron-atom ratio at the phase boundary, with the not-quite-so-large band gaps measured by optical data. In order to fix these ambiguities, clear-cut experimental evidence which indicates the shape and the size of the Fermi surface in alloys is required.

Recently the problem of the stabilization of long-period superlattices in alloys has been treated by the present authors.[5] It turned out that the analysis of the result indicated, in a clear-cut way, the existence of a Fermi surface which is similar to that of pure noble metals in shape and size. In some alloys having an ordered face-centered cubic structure, antiphase structures with a definite domain size exist, and it is found that the domain size changes continuously

over a wide range depending on the electron-atom ratio. The dependence of the period upon the electron-atom ratio is explained in such a way that the Fermi surface touches the newly formed superlattice Brillouin zone boundaries {110}, the size of which is adjusted by the existence of the extra period depending on the electron-atom ratio in a way shown in Fig. 1. Here we show the cross section of the separated {110} Brillouin zone boundaries, the separation being due to the existence of the superperiod, in the plane through the origin and parallel to the (001) plane, and the inscribed Fermi sphere. More exactly, it is a hypothetical sphere, the size of which is proportional to the actual Fermi surface. In alloys with a one-dimensional long-period superlattice, such as CuAu II with additional elements, Cu-Pd, Cu-Pt, Au-Cd, Ag-Mg, Au-Zn, etc., the dependence of the domain size M (half period) upon the electron-atom ratio e/a is given by the following formula:

$$e/a = (\pi/12\, t^3)(2 \pm 1/M + 1/4M^2)^{3/2}. \qquad (1)$$

Here t is a truncation factor which indicates the effective size of the Fermi sphere in the [110] direction as compared with the free-electron sphere value. In an actual case, t is determined from the fitting of the theoretical curve [Eq. (1)] to the data. The plus or minus sign in Eq. (1) indicates that the touching of the Fermi sphere occurs at either the outer or inner zone boundaries of Fig. 1 depending on the size of the Fermi sphere, in other words, on whether the electron-atom ratio is larger or smaller than the critical value $(e/a)_c$. The result of the analysis on the alloys mentioned above is shown in Table I. The
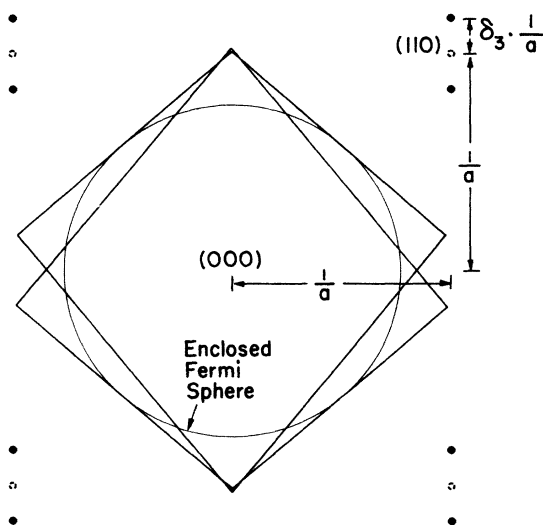

FIG. 1. A cross section of the Brillouin zone of a one-dimensional long-period superlattice in a face-centered cubic alloy, in a plane through the origin and parallel to the (001) plane, showing the separation of the {110} boundaries. The superperiod exists in the k_y direction.

Table I. Summary of data on one-dimensional long-period superlattices.

Alloy series	Composition range (at. %)	$e/a - (e/a)_c$ [a]	Truncation factor t
Cu-Pd	20-26% Pd	–	0.941
Cu-Pt	24-26% Pt	–	0.958
Au-Cd	24.6-25.5% Cd	+	0.950
Ag-Mg	22-28% Mg	+	0.962
Au-Zn	21-29% Zn	+	0.950
Cu-Au	(a) 40-55% Cu	+	0.950
	(b) CuAu II plus additional elements	+	0.950

[a] The critical value of the electron-atom ratio.

important fact is that the values of t come out to be almost the same (about 0.95) irrespective of the kind of alloy or of the value of the electron-atom ratio. This fact indicates that the effective size of the Fermi sphere in the [110] direction is approximately 0.95 of the size of the free-electron sphere in all alloy series of the noble metals shown in Table I.

In light of the present knowledge of the Fermi surface of pure noble metals, the above result can be explained in the following way. The Fermi surface bulges out in the [111] direction and touches the {111} boundaries, forming necks. Since the diameter of the neck is small, it leaves a reasonably spherical surface around the [110] direction where the actual stabilization takes place. Because of the existence of the necks, the effective diameter is reduced. The value of 5% given by the analysis does seem to be larger than the value expected from the measurement of the difference in the period of the belly orbit obtained from the de Haas—van Alphen effect measurements from that of the free-electron sphere value.[6] Actually the volume of the necks obtained from experiment only amounts to, at most, 2% of the free-electron sphere. However, the shape of the remaining Fermi surface is not quite spherical and measurements of the magnetoacoustic effect,[7] which calipers the Fermi surface, indicate that the diameter of the Fermi surface of these metals in the [110] direction is actually smaller than the free-electron value by four or five percent. Recent theoretical calculations also indicate this contraction in the [110] direction.[8] Also, if we think of the actual distortion of the Fermi sphere at the zone boundary which presumably takes place at the condition of the maximum stabilization, the value of 5% still seems quite reasonable. A schematic figure showing this possible distortion and the partial origin of the truncation factor is shown in Fig. 2. The fact that we can predict the period of the long-period superlattice with a reasonable value of the size of the Fermi surface shows not only that the above interpretation is quite reasonable, but also that the Fermi surface, which is similar to that of noble metals in shape and in size, definitely exists in these alloys.
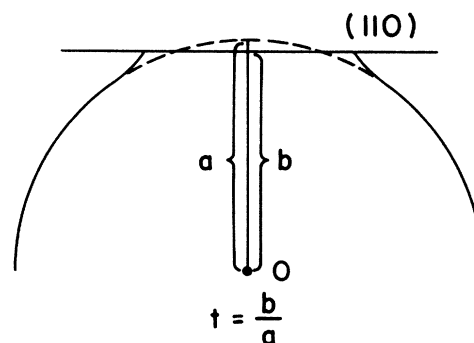

FIG. 2. A schematic drawing showing the possible relation of the Fermi surface and the Brillouin zone boundaries, and the partial origin of the truncation factor.

At the same time, the constancy of the truncation factor with the change of the e/a ratio in the same alloy series or similar values of t for different alloy systems indicate that the general shape of the Fermi surface remains proportionately constant even if the size of the Fermi surface changes. This is especially striking for alloys with small e/a ratios such as Cu-Pd or Cu-Pt alloys in which the size of the Fermi surface is small and the neck cannot be expected to touch the {111} boundaries.

[1]The Fermi Surface, Proceedings of an International Conference at Cooperstown, New York, edited by W. A. Harrison and M. B. Webb (John Wiley & Sons, Inc., New York, 1960).

[2]H. Jones, Proc. Phys. Soc. (London) 49, 250 (1937). Also N. F. Mott and H. Jones, Theory of the Properties of Metals and Alloys (Clarendon Press, Oxford, 1936).

[3]M. H. Cohen and V. Heine, Advances in Physics, edited by N. F. Mott (Taylor and Francis, Ltd., London, 1958), Vol. 7, p. 395; V. Heine, reference 1, p. 279.

[4]W. Hume-Rothery and D. J. Roaf, Phil. Mag. 6, 55 (1961).

[5]H. Sato and R. S. Toth, Phys. Rev. 124, 1833 (1961); also H. Sato and R. S. Toth (to be published).

[6]D. Shoenberg, Phil. Mag. 5, 105 (1960).

[7]R. W. Morse, reference 1, p. 214; R. W. Morse, A. Myers, and C. T. Walker, J. Acoust. Soc. Am. 33, 699 (1961).

[8]B. Segall, Phys. Rev. Letters 7, 154 (1961); Phys. Rev. 125, 109 (1962). G. A. Burdick, Phys. Rev. Letters 7, 156 (1961).