Fermi-surface radii in copper, silver, and gold

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(Received 2 February 1982)

New Fourier expansions for the Fermi-surface radii of copper, silver, and gold have been obtained on the basis of high precision de Haas–van Alphen data. The radii agree with the values quoted by Halse to better than 0.2% except for gold near the ⟨100⟩ direction, where the Halse values are about 0.6% too large.

The Fourier-series expansions for the Fermi surfaces of copper, silver, and gold given by Halse[1] have been used extensively for determining radius vectors on the Fermi surfaces. Recently Steele and Goodrich[2] have measured some radii in Au using the radio-frequency size effect (RFSE) and, finding discrepancies of 1–2% for most of the radii, suggest that new Fourier expansions using high-precision de Haas–van Alphen data should be obtained. The purpose of this paper is to point out that such expansions exist and that even in gold the radii generally agree well with Halse's values.

The fits of Halse were made prior to the publication of high-precision de Haas–van Alphen data by Coleridge and Templeton (CT).[3] In that paper parameters for a new set of five coefficient expansions are listed. These fits were developed primarily for considering area changes induced by alloying and were obtained by fitting six areas in a least-squares sense. They have the failing that the neck radii, inherently the most accurate and most easily fitted feature of the Fermi surfaces, are fitted rather poorly. However, as previously noted,[4] the system of equations involved in the least-squares fitting procedure is not well-conditioned so caution is needed in expanding the fit to six, let alone seven, independent coefficients. An approach found to be satisfactory was to keep the first two coefficients fixed and adjust the remaining five terms to fit the neck area exactly and improve the agreement with the other areas. The coefficients for these seven term fits are listed in Table I. The improved agreement with the experimental data and the correct volume of the Fermi surfaces indicates that although these fits have only five adjustable parameters, the extra Fourier components included result in improved representations of the Fermi surfaces.

Rather than listing radii in detail, a few selected values along symmetry lines are compared in Table II with the corresponding values from Halse. A check on the reliability of the inversions can also be obtained by looking at the results of a completely different kind of fit, e.g., a nonrelativistic Korringa-Kohn-Rostoker (KKR) parametrization. For this a convenient choice is the fits of Shaw, Ketterson, and Windmiller (SKW).[5] These did not use the high-precision de Haas–van Alphen data of Ref. 3 but in the cases of Cu and Ag agree well with parametrizations which do use that data.[6] For Au the agreement is not quite so good, so another KKR parametrization,[7] fitted to the high-precision data, is also listed.

It is apparent from Table II that in most cases the radii shown are in good agreement and this is true for all radii except in Au near the ⟨100⟩ direction. With this exception the Halse radii can be considered accurate to better than 0.2%. For

TABLE I. Coefficients for seven term fits (Halse notation). Also shown are the volume of the Fermi surface and the rms deviation of the fits from the experimental areas in units of 10^{-5} of the free-electron cross section.

	C_0	C_{200}	C_{211}	C_{220}	C_{310}	C_{222}	C_{321}	Volume	rms error
Copper	1.691 3140	0.006 574	−0.422 661	−0.017 235	−0.054 863	−0.005 457	0.014 955	1.000 00	1.3
Silver	−0.898 274	−0.120 718	−0.902 220	−0.141 998	−0.105 983	−0.002 707	0.011 181	1.000 07	1.7
Gold	−2.263 657	−0.167 472	−1.248 022	−0.102 381	−0.171 449	−0.020 910	0.040 982	1.000 66	11.0

TABLE II. Fermi-surface radii in the noble metals from various fits in units of $2\pi/a$.

	⟨100⟩	⟨110⟩	⟨211⟩	Neck (mean)
Copper				
Halse Cu 7[a]	0.8279	0.7431	0.7829	0.147 37
CT Cu 5VI[b]	0.8291	0.7431	0.7828	0.146 36
CT Cu 7[c]	0.8268	0.7429	0.7825	0.147 37
SKW[d]	0.8269	0.7432	0.7825	0.147 36
Silver				
Halse Ag 7[a]	0.8182	0.7532	0.7808	0.106 65
CT Ag 5IV[b]	0.8210	0.7530	0.7808	0.1054
CT Ag 7[c]	0.8192	0.7530	0.7807	0.106 65
SKW[d]	0.8196	0.7530	0.7804	0.1067
Gold				
Halse Au 5[a]	0.8837	0.7366	0.7782	0.139 62
CT Au 5VI[b]	0.8807	0.7365	0.7778	0.1376
CT Au 7[c]	0.8777	0.7361	0.7774	0.139 56
SKW[d]	0.8777	0.7369	0.7780	0.139 65
C[e]	0.8794	0.7376	0.7773	0.139 56

[a]Reference 1.
[b]Reference 3.
[c]Table I of this work.
[d]Reference 5.
[e]Reference 7.

all inversions the ⟨100⟩ radius vector is the least accurately determined but nevertheless, from the agreement of the various new fits, it is fairly clear that the Halse values in Au are about 0.6% too large for radii near ⟨100⟩. The discrepancy along this direction does not explain the results of Steele and Goodrich; indeed, using radii from the new inversions increases the discrepancies near ⟨100⟩ rather than reducing them. It should be noted that although mean values of the neck radii are listed in Table II all inversions are in agreement that the anisotropy in the necks is at the most 0.1%. Furthermore, for radii near the neck, de Haas–van Alphen inversion schemes are least likely to be in error because the radius, measured from the center of the zone, can be deduced from just the neck cross section and the dimensions of the Brillouin zone. It seems clear, therefore, that the discrepancy between RFSE and de Haas–van Alphen Fermi-surface radii in Au is not associated with errors in the Halse expansions of de Haas–van Alphen data.

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