reasonable, when compared with the recent data of Reed and Condon,[7] than earlier estimates of $B_0 \gtrsim 100$ kG. Finally, the orientation dependence of the SdH frequency was found to agree well with dHvA results, in contradiction to recent results in the literature.

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*Present address: Xerox Corporation, Rochester, N. Y.

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Comments on Pseudopotential Form Factors for White Tin

M. A. C. Devillers and A. R. de Vroomen
Fysisch Laboratorium, Katholieke Universiteit, Nijmegen, The Netherlands

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While preparing for an experimental investigation of electron-phonon mass enhancement and relaxation times in white tin, we were confronted with large inconsistencies in the published form factors for this metal.[1-5] In this paper we are presenting the results of calculations that should clarify this matter a great deal.

The experiments on which our calculations are based are Fermi-surface calipers obtained from very accurate rf size-effect measurements.[6] With a plane-wave matrix, large enough to assure convergence with respect to the number of reciprocal lattice vectors, we fitted the four form factors $V(K_n)$, $K_n < 2k_F$, and the Fermi energy (or mass) at 14 selected points, representative of the Fermi surface. The best fit is obtained for $E_F = 2.11$ (throughout this paper, we use $h^2/2ma^2$ as unit of energy) [Fig. 1(a)]. Compared with the nearly-free-electron value $E_{\mathrm{NFE}} = 2.312$, this suggests a Fermi-surface-band effective mass of about $0.92m_0$. For the best energy value the fit shows a rms deviation in the calipers of about $0.004k_0$ ($k_0 = \Gamma L = 2\pi/a$), which is slightly larger than the experimental inaccuracies. In Fig. 1(a) one sees that this Fermi energy can be determined to within 0.01 (our units).

Our fitted form factors show a large energy dependence [Fig. 1(b)]. We are confident that these curves are representative of the entire Fermi surface, rather than of the specific sample of data points.

In the following we shall compare our results with previous calculations. The work of Weisz[1] was based on Gantmakher's pioneering rf size-effect data. Due to some uncertainties in the line shape the inaccuracy of Gantmakher's calipers amounts to several percent. Weisz found a best Fermi energy of about 2.24 (our units). For this energy we find a fit which has a rms deviation seven times larger than that of our best fit. We feel that Weisz's deviation from our results is due to the large limitation in accuracy and in the number of his data points.

Stafleu and de Vroomen[2] took E_F equal to the free-electron value and used a "few-plane-wave" matrix. In view of their aim to obtain a rough agreement with their de Haas–van Alphen (dHvA) experiments the discrepancies with our results are reasonable.

Craven's results[3] are of more serious concern to us. He claims to describe to within 1% the accurate dHvA measurements of Craven and Stark[7] by form factors, given in Fig. 1(b), at an energy $E_F = 2.34$ (our units). However, his interpolated

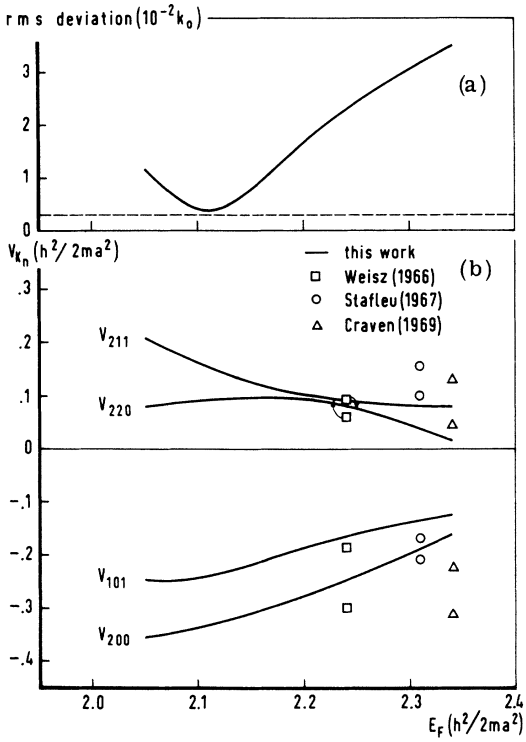

FIG. 1. (a) rms deviation between calculation and experiment of the four-parameter fit to the Fermi surface of white tin as a function of the Fermi energy (solid line). The broken line indicates the mean experimental inaccuracy. The value of the lattice constant a is 5.812 Å. (b) Four Fourier transforms of the pseudopotential, fitted to the Fermi surface of white tin as functions of the Fermi energy.

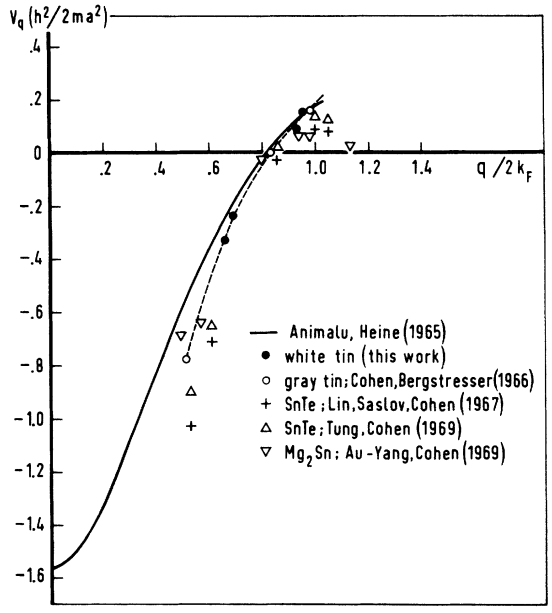

FIG. 2. Pseudopotential form factor for tin.

Fermi-surface deviates appreciably from Matthey's data[6] and our best interpolated Fermi surface. Therefore, it seems that one should be very careful in calculating pseudopotential form factors from dHvA data.

Another point relating Craven's form factors and not necessarily related to the above comments is that if his form factors were, for some reason, wrong by a factor of exactly 2, excellent agreement with our form factors at Craven's energy appears. This might be due to a scaling error.

Turning to the Cohen and Bergstresser's[5,8] form factors, evaluated from gray tin data, it is possibly accidental (see Cohen and Heine,[8] however) that their form factors and ours at our best E_F lie on the same smooth curve (Fig. 2). The form factors for tin, obtained from optical data on SnTe[8-10] and Mg_2Sn,[8,11] are also presented in Fig. 2.

The agreement with the Animalu-Heine[4] model potential form factors is as good as is encountered in other metals.

In conclusion, discrepancies between published form factors for white tin and our present ones can be traced back to inadequacies of Fermi-surface input data used in calculating the form factors. Stated more positively, Fermi-surface geometry data of reasonable accuracy, if properly treated, can provide us with form factors and Fermi energy accurate to about $\frac{1}{2}\%$ of E_{NFE}.

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