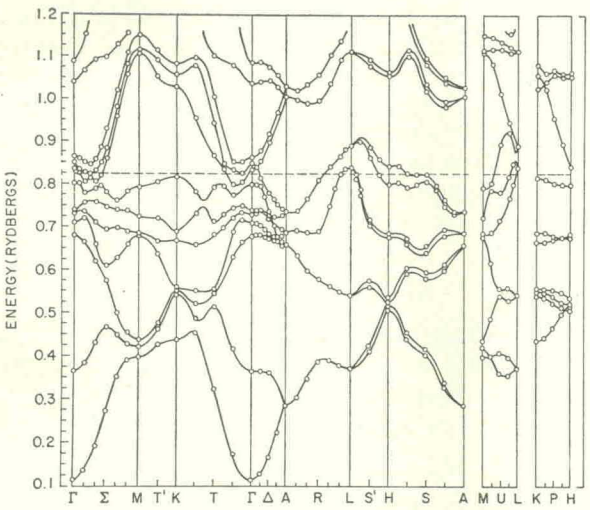


FIG. 13. The relativistic energy bands for rhenium, including the effects of spin-orbit coupling (from Ref. 19).

In principle, we should be able to distinguish between the two possible critical points ($S_2$ or minimum) from the shape of the pressure dependence of $(\partial T/\partial P)_{\text{nonlinear}}$. However, in the present case of rhenium and its alloys, the shape is too ill-defined to make any such distinction. Fortunately, it is possible to make at least a rough qualitative comparison with the height and width of the curves calculated by Makarow and Bar'yakhtar.[4] These authors showed that

$$\Delta T/T_c \sim (k\Theta_D/E_F)^{1/2}, \tag{3}$$

and that the minimum half-width of $(\partial T_c/\partial E_F)_{\text{nonlinear}}$ as a function of energy, is $\sim k\Theta_D$ (see Fig. 10). In Table II, we compare the estimated values of these quantities with the observed values both for rhenium and thallium. The estimate of the half-width energy of the maximum in $(\partial T_c/\partial E_F)_{\text{nonlinear}}$ was obtained from the relationship

$$\Delta E \sim c\Delta z/2N_b(E), \tag{4}$$

where $N_b(E)$ is the band density of states and $c$ is the alloying addition of valence difference $\Delta z$ required to move $P_c$ by a half-width of the maximum in $(\partial T_c/\partial P)_{\text{nonlinear}}$. It can be seen that the contribution to $T_c$ is of the correct order of magnitude in both cases. Reasonable agreement is obtained for the estimate of the energy spread of $(\partial T_c/\partial E_F)_{\text{nonlinear}}$ from alloying and that obtained from $\Theta_D$ for Tl, but a serious discrepancy is found for Re.

TABLE II. A comparison of the calculated and observed parameters associated with a nonlinear contribution to $T_c$ for rhenium and thallium.

| | Half-width of $\left(\frac{\partial T_c}{\partial E_F}\right)_{\text{nonlinear}}$ meV | | $\frac{\Delta T_c}{T_c}$ | $\left(\frac{k\Theta_D}{E_F}\right)^{1/2}$ |
|---|---|---|---|---|
| | $k\Theta_D$ | Measured | | |
| Re | 44 | 2 | 0.03 | 0.06 |
| Tl | 8 | 5 | 0.06 | 0.03 |

Support for our model of a change in Fermi-surface connectivity is found in the band structure and Fermi-surface calculations for rhenium by Mattheiss.[19] The results of his calculation for the relativistic energy bands, including the effects of spin-orbit coupling are shown in Fig. 13. It can be seen that flat regions in the $E(\mathbf{k})$ curves occur close to the Fermi surface in the eigth zone along the direction AH and in the ninth zone along the directions $\Gamma K$ and $\Gamma M$. Mattheiss pointed out that the detailed nature of the Fermi surface in these regions is very sensitive to the value of $E_F$ and he illustrated the changes in topology which would occur if the Fermi energy were increased by $\sim$70 meV. Thus, he showed (Fig. 14) that necks appear in the electron sheets ($e_8$ and $e_9$) in the eighth and ninth zones.

Using the elastic-constant data of Shepard and Smith[20] for rhenium, we calculate that a hydrostatic pressure of 20 kbar does not change $c/a$ by more than 0.05% at 4.2°K. Thus, since the compression is isotropic to obtain the necessary changes in the relative energies of the flat regions of the $E(\mathbf{k})$ curves and the Fermi energy requires strong hybridization of the wave functions. It is therefore of considerable interest to

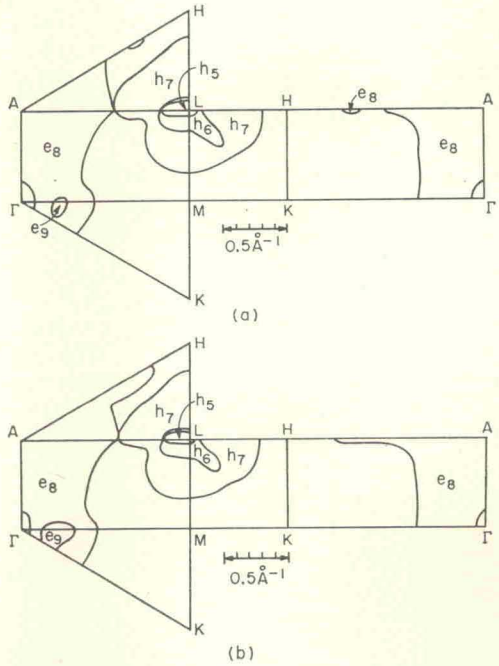


FIG. 14. Intersection of the rhenium Fermi surface with symmetry planes of the hexagonal Brillouin zone. The $e_8$ and $e_9$ represent electron sheets in the eighth and ninth zones. The results in (a) correspond to a Fermi energy of 11.22 eV. The corresponding results in (b) indicate the changes which occur when the Fermi energy is raised by 68 meV (from Ref. 19).

[19] L. F. Mattheiss, Phys. Rev. **151**, 450 (1966).

[20] M. L. Shepard and J. F. Smith, J. Appl. Phys. **36**, 1447 (1965).

examine the degree of admixture in the wave functions in the eighth zone along AH and in the ninth zone along $\Gamma K$ and to calculate the change in energy of these bands with change of volume. It is an interesting aside that these effects would not have occured in the absence of spin orbit coupling in rhenium.

*Note added in proof.* Since this paper was written, an article by Higgins and Kaehn has been published [Phys. Rev. **182**, 649 (1969)] in which the effect of impurity broadening on the singularities in the electron density of states and the superconducting transition temperature, associated with the passage of the Fermi energy through a critical point, was investigated. These authors report that the structure in $T_c$ as a function of Fermi energy is broadened by the order of $kT_c$ for pure metals ($\sim$4°K in the particular case of In which they consider), whereas for In with 2% Cd the impurity broadening is $\sim$50°K. However, since the effect of the electron-phonon interaction is to average the density of states over a region $\pm k\Theta_D$ about the Fermi energy, any structure in $T_c$ as a function of energy must be broadened over an energy of $2\Theta_D$, or $\sim$200°K in the case of In. This is clearly seen in Fig. 9.

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