Letters

On the Fermi Surface of Disordered Cu_3Au

Above the critical temperature (390° C), the alloy Cu_3Au exists in the disordered state. In this state, it is face-centred cubic. Below 390° C, an ordered, simple-cubic structure is formed. The transformation from the disordered to the ordered state is accompanied by changes in a large number of properties. These changes can be used to obtain information regarding the electronic structure of the alloy. We have been interested in the galvanomagnetic properties of Cu_3Au, in both the ordered and disordered states. We describe here a study of the Fermi surface in the disordered alloy.

The Hall coefficient and the magnetoresistance were measured in the disordered Cu_3Au. The experimental details were fairly standard and will not be described here. Table I shows the results where the free-electron values have also been included. Also in table I are collected some other properties which can be directly related to the electronic structure.

In spite of several attempts, we could not clearly detect a transverse magnetoresistance effect (referred to hereafter simply as "magnetoresistance") above the noise level (change in resistance per unit resistance of the order of 10^{-5}). This indicates that the magnetoresistance is exceedingly small even at liquid-nitrogen temperature and in a magnetic field of 18.6 kgauss. This observation seems to be in disagreement with the magnetoresistance measurements on disordered Cu_3Au of Komar [1]. However, this may be due to the fact that Komar used an alloy which was quenched from 386° C and therefore the alloy could have been in a partially ordered state.

Magnetoresistance is caused by a departure from the free-electron behaviour, i.e. if the Fermi surface is spherical and the electron relaxation time is isotropic, magnetoresistance will be zero. A non-zero magnetoresistance, therefore, implies either a distortion of the Fermi surface and/or an anisotropy of the relaxation time. The relaxation time in the disordered Cu_3Au, in comparison to that in Cu (or Au), will be fairly isotropic, owing to the absence of long-range order.* Therefore, throughout our discussion, we assume an isotropic relaxation-time for the disordered Cu_3Au.

From the present magnetoresistance data, therefore, we conclude that a fairly spherical Fermi surface exists for the disordered Cu_3Au. This is further supported by the data on the Hall effect, electronic specific heat and thermoelectric power: the observed values for disordered Cu_3Au, as compared to those for Cu and Au, are nearer to the free-electron values (see ratios of the observed to the free-electron values in table I). Our conclusion regarding the Fermi surface of the disordered Cu_3Au is also in accord with the results of Flinn *et al* [2]. These authors measured the elastic constants for ordered and disordered Cu_3Au from 4.2 to 300° K. From the low temperature data for the disordered state, Flinn *et al* concluded that the Fermi surface becomes more spherical on alloying Cu with Au.

A fair amount of experimental evidence is available to show that there is some truth in the Cohen and Heine theory, i.e. the sphericising of the Fermi surface due to alloying. The electronic specific heat of disordered Cu_3Au seems to be in reasonable agreement with this theory [3]. Furthermore, the magnetoresistance and the thermoelectric power data also show a behaviour expected on the basis of Cohen and Heine's theory, in the sense that, to explain these observations, a less anisotropic Fermi surface than that of either Cu or Au is required.

The above conclusion regarding the Fermi surface is in conflict with the view of other investigators. Von Neida and Gordon [4] considered the Hall effect in the disordered alloy and indicated that the Fermi surface in the disordered state might be similar to that of Cu. Airoldi *et al* [5] studied the thermoelectric power of the ordered and disordered Cu_3Au. They observed that the thermoelectric power is positive in the case of the disordered alloy, as for Cu and Au, although much smaller in magnitude. This is in contrast to the ordered alloy, where thermoelectric power is negative. From this observation, Airoldi *et al* also suggested that the Fermi surface of the disordered Cu_3Au

*If we extend the idea of Erez and Rudman [12] to Cu_3Au, the scattering due to the atomic distribution – i.e. due to the order-disorder effects – will be dominant over the electron-phonon scattering (since in Cu_3Au $\tau_p/\tau_c \simeq 1.5$, where τ_p is the relaxation time for electron-phonon scattering and τ_c that due to the atomic distribution).

TABLE I Electronic properties of Cu, Au, and disordered Cu_3Au.

Property	Copper (Cu)	Gold (Au)	Disordered* Cu_3Au
Hall effect			
$R_H \times 10^{12}$ (ohm cm/gauss) at room temperature			
Observed R_{H0}	−0.52 [9]	−0.72 [9]	−0.67
Free-electron R_{Hf}	−0.74 [9]	−1.06 [9]	−0.82
R_{H0}/R_{Hf}	0.70	0.68	0.81
Magnetoresistance			
At liquid-nitrogen temperature and 18.6 kgauss	$>10^{-5}$ [10]	$>10^{-5}$ [10]	$\sim 10^{-5}$
Thermoelectric power			
$Q \times 10^6$ (V/° C) at 0° C			
Observed Q_0	+1.73 [11]	+1.85 [11]	~ +0.4 [5]
Free-electron Q_f	−2.9 [11]	−3.7 [11]	−3.07
Q_0/Q_f	−0.59	−0.50	−0.13
Specific heat (electronic)			
$\gamma \times 10^3$ (joule/mol. ° C²)			
Observed γ_0	0.688 [9]	0.743 [9]	0.66 ± 0.02 [8]
Free-electron γ_f	0.502 [9]	0.644 [9]	0.738 [8]
γ_0/γ_f	1.37	1.15	0.89

*75.5 at. % Cu: quenched from 480° C.

might be similar to that of Cu or Au, i.e. Fermi surface touching the Brillouin zone boundaries in <111> directions. However, this conclusion is not sufficiently justified in view of the contradictory results of Nagy and Toth [6], who reported a negative thermoelectric power for the disordered alloy at room temperature. A positive Hall effect is usually interpreted in terms of the predominance of "hole" conduction. The same argument can be applied to the thermoelectric power. But the thermoelectric power effects are rather complicated, and a positive thermoelectric power can also be due to effects other than hole conduction. Jones [7] has shown that a positive thermoelectric power does not necessarily mean that the Fermi surface touches the Brillouin zone boundaries. The positive sign can also be explained if the Fermi surface is close to the zone boundary.

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