Electron topological transitions in the Mo–Re system

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The electron spectrum and thermodynamic properties of disordered solid solutions $Mo_{1-x}Re_x$ are analyzed in the approximation of a coherent potential. Two electron topological transitions are found, at $x \sim 0.02$ (this is the formation of a new electron cavity on the Fermi surface) and at $x \approx 0.08$ (the formation of a bridge). © *1994 American Institute of Physics.*

Experiments on disordered alloys of the Mo–Re system have revealed structural features on the concentration dependence of physical properties.[1,2] Ignat'eva and Cherevan'[1] observed a nonlinear dependence of the superconducting transition temperature under pressure, and Velikodnyĭ *et al.*[2] observed a giant anomaly in the thermal emf of the alloy $Mo_{1-x}Re_x$ with $x \sim 0.11$. These investigators[1,2] attributed the occurrence of these features to an electron topological transition: the creation, at $x \sim 0.11$, of a new electron cavity of the Fermi surface on the NH axis of the Brillouin zone. That explanation was based on data on the electron spectrum of pure molybdenum[3] and simple estimates in a rigid-band model. Nevertheless, a definitive conclusion regarding the occurrence of an electron topological transition in a disordered alloy cannot be reached until the electronic structure has been studied. Attempts have been made in this direction for the Mo–Re system. Yarmoshenko *et al.*[4] reported observing a van Hove singularity at $x \sim 0.1$ in x-ray photoemission measurements, but their calculation of the density of states in the strong-coupling model revealed no structural features in the electron spectrum. We thus have no reliable information on the electronic structure of the Mo–Re alloys at the moment.

In this letter we offer a theoretical analysis of the electron spectrum and the possibility of an electron topological transition in alloys of the Mo–Re system. The alloys $Mo_{1-x}Re_x$ form a continuous series of disordered solid solutions up to $x \sim 0.3$. The electron spectrum and thermodynamic properties of disordered solid substitution solutions of rhenium in molybdenum are calculated "from first principles" in the approximation of a coherent potential. In the approximation of a coherent potential,[5] the disordered alloy is replaced by a lattice of effective scatterers. The parameters of the effective medium are chosen in such a way that the random distribution of various atomic species on the lattice makes no contribution to the scattering, on the average. In the method used here, the one-particle electron Green's function and its spectral density (required for constructing the Fermi surface) are found by the self-consistent density-functional method in a basis of linear MT orbitals (see Refs. 6 and 7 for more details on the method). The spectral density is calculated with $x = 0.02$ and above; the thermodynamic properties are calculated for $x \geqslant 0.04$.

First, we found that a new electron cavity forms at $x < 0.02$ (not at $x \sim 0.1$, as has

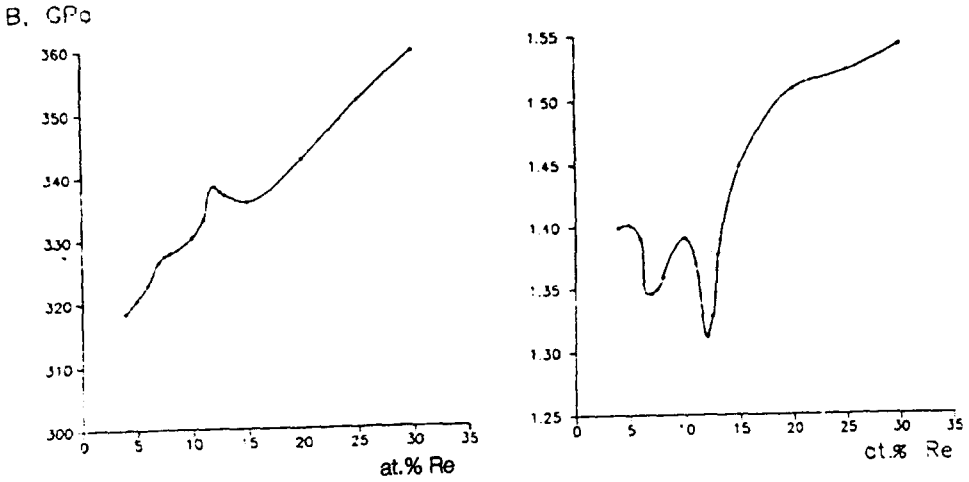

FIG. 1. Concentration dependence of (a) the bulk modulus and (b) the Grüneisen constant of a disordered Mo–Re alloy.

been proposed previously[1,2]). (This cavity was to be expected, since in pure molybdenum there is a minimum of an unfilled electron band 0.02 eV above the Fermi level near the NH axis.) At $x \sim 0.02$ there are already two clearly defined peaks in the spectral density at $\epsilon = E_F$ on the NH line. This aspect of the behavior of the thermodynamic properties cannot be observed because of the insufficient accuracy of the calculations of these properties at $x \leqslant 0.04$.

There are two structural features in the thermodynamic properties calculated in the interval $0.04 \leqslant x \leqslant 0.3$: at $x \sim 0.08$ and ~ 0.12 (Fig. 1). The first can confidently be linked with an electron topological transition resulting from the formation of a bridge in the ΓNH plane. In the first place, the bulk modulus on the side of higher connectedness of the Fermi surface has a characteristic square-root singularity, as it should for an electron topological transition of this type.[8] The Grüneisen constant tends toward infinity (but does not actually become infinite, because of a smearing of the transition due to the disorder). Second, an electron topological transition is indicated unambiguously by the change in the profile of the spectral density with the concentration. [This profile was measured along a line parallel to NH and lying a distance of $0.57(2\pi/a)$ from it, i.e., passing through the point at which the bridge forms.] In a disordered alloy, a finite lifetime of an electron state with a certain energy leads to a "smearing" of the energy levels of the electron. The characteristic smearing of each level is $\Gamma \sim \hbar/\tau(\epsilon)$, where $\tau(\epsilon)$ serves as the average lifetime of an electron with an energy ϵ. In particular, the Fermi surface is also smeared; as a result, the electron topological transition stretches out over an interval of concentrations[9] (see the review of results in Ref. 10). As can be seen from Fig. 2, the behavior of the spectral density ideally corresponds to the concept of a smeared Fermi surface. To simplify the discussion, we replace a Gaussian smearing of the Fermi level by a profile with sharp boundaries: from $E_F - \Gamma/2$ to $E_F + \Gamma/2$. In this case

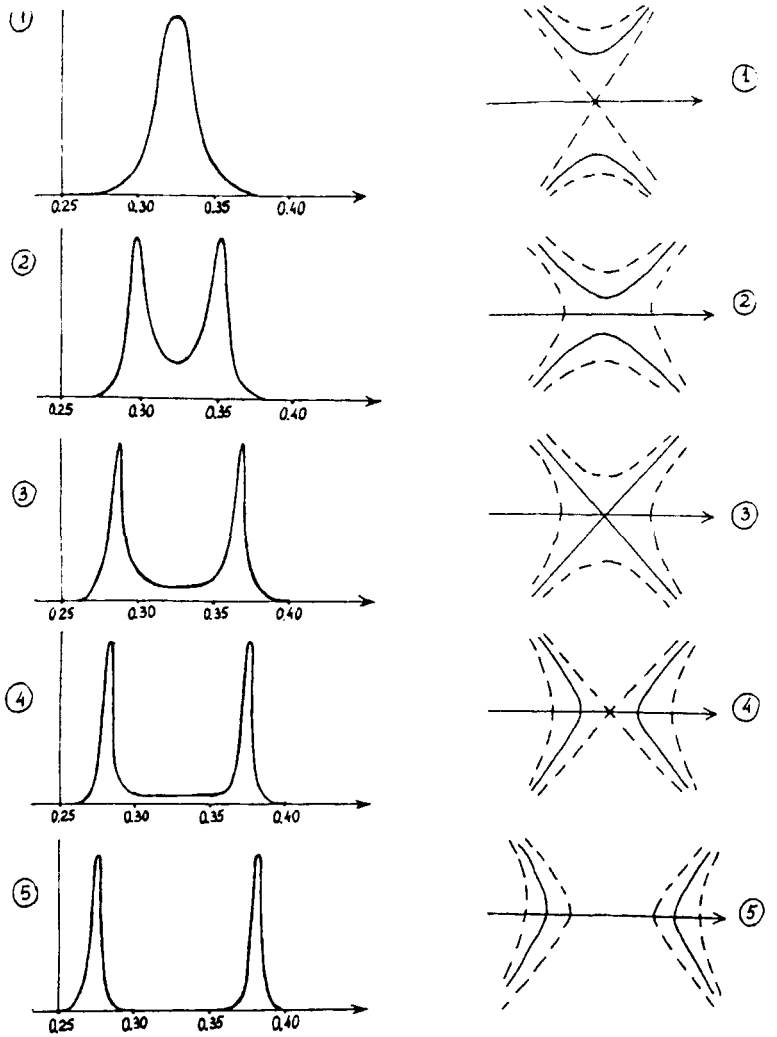

FIG. 2. a: Profiles of the spectral density at the Fermi surface along the straight line parallel to NH and passing through the point at which the bridge forms. The distance from the ΓH line is plotted along the abscissa. 1—3 at. % Re; 2—5%; 3—8%; 4—11%; 5—15%. b: Fermi surfaces corresponding to these concentrations near the point at which the bridge forms. The horizontal straight line corresponds to the line along which the profiles of the spectral density are calculated. Solid curves) "Actual" (unsmeared) Fermi surface; dashed curves) schematic representation of the smearing due to impurities. The "midpoint" of the transition corresponds to a transition of 8 at. % Re.

(for example), the "beginning" of the electron topological transition corresponds to the case in which smeared Fermi surfaces of this sort first touch; on the curve of the spectral density, this touching means the appearance of a peak. This peak then rises and begins to split in two. This splitting occurs at the concentration $x_c = 0.08$, which corresponds to the formation of a bridge on the Fermi surface proper (the unsmeared surface). The "end" of

the transition corresponds to the ultimate separation of the profile of the spectral density into two distinct peaks.

This behavior of the spectral density is itself evidence that an electron topological transition of the "bridge-creation" type occurs. However, this picture also agrees very well with the calculated concentration dependence of physical properties: The "midpoint" of the transition, i.e., the position of the maximum of the Grüneisen constant (for example), corresponds to the concentration x_c, and the smearing, determined from the half-width of the peak, corresponds to the picture of a change in the spectral density with the concentration.

Finally, the feature at $x \sim 0.12$ evidently is unrelated to the electron topological transition, since the behavior of the spectral density does not indicate any change in the topology of the Fermi surface out to the stability boundaries of the solid solution. This feature is probably associated with the peak structure in the density of states; this situation should of course affect characteristics integrated over the spectrum.

In summary, two electron topological transitions occur in alloys of molybdenum with rhenium in the region $x \leqslant 0.3$: the formation of an electron cavity at $x \sim 0.02$ and the formation of a bridge at $x \sim 0.08$. These conclusions do not contradict the experimental results of Ref. 2: The peak in the thermal emf, with the asymmetry characteristic of an electron topological transition, is fairly wide despite being local, and its wing at $x \approx 0$ lies well above the value of the thermal emf for pure molybdenum. This peak spans two closely spaced transitions, which are difficult to separate in this experiment, because the Fermi surface is smeared by the disorder of the alloy, and also because of the temperature. With regard to the nonlinear pressure dependence of T_c (if it is indeed associated with the electron topological transition), we note that it is observed at values as low as $x \sim 0.06$, according to Ref. 1.

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