shows that in the neighborhood of the magnetic axis of a Tokamak-type configuration, ballooning modes are stabilized simultaneously with localized modes. This result is surprising since in the case of magnetic surfaces with circular cross section the localized criterion does not yield[5] a critical β. Indeed, the calculations of Adam and Mercier[7] have recently been completed[8] by taking into account second-order corrections in the curvature and it was shown that the stability limit is practically given by $\iota/2\pi<1$. Hence, it seems that a critical β may perhaps be found only for perturbations with small values of m and a radial extension on the scale of the plasma radius.

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MODEL TO EXPLAIN LARGE CHANGES IN THE ELECTRONIC DENSITY OF STATES WITH ATOMIC ORDERING IN V_3Au

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The superconducting transition temperature of V_3Au has been experimentally shown to vary by a factor of 300, depending on the degree of atomic ordering. This has previously been attributed to a change in the electronic density of states $n(E)$ with ordering. A model is proposed here which provides a theoretical basis for this change in $n(E)$ with ordering.

Previous publications[1-3] have shown that the increase in T_c for the compound V_3Au by a factor of almost 300 is caused by atomic ordering. A study of the NMR properties[4,5] has shown that this change in T_c is accompanied by a change in the core-polarization term of the total Knight shift. This term, relatable to the d electrons, suggested an increase in the d-band density of states at the Fermi level, $n(E)$, with increasing superconducting transition temperature. We present here a model which theoretically predicts this increasing density of states with atomic ordering in V_3Au.

Figure 1 shows the observed temperature dependence of the Knight shift (above T_c) for a single V_3Au sample with varying T_c values caused by changing its degree of atomic ordering. With increasing T_c, two features are immediately obvious: First, the total Knight shift decreases at 4.2 K, and secondly, the total Knight shift shows an increasing temperature dependence. In Ref. 4 (hereafter R4), it was shown that both of these features are explicable when based on an increasing d-electron density of states at the Fermi level. Additionally, results shown in Figs. 3 and 5 of R4 were cited as further experimental proof[6] of the postulated increase in $n(E)$. Although it was clear that atomic ordering was causing an

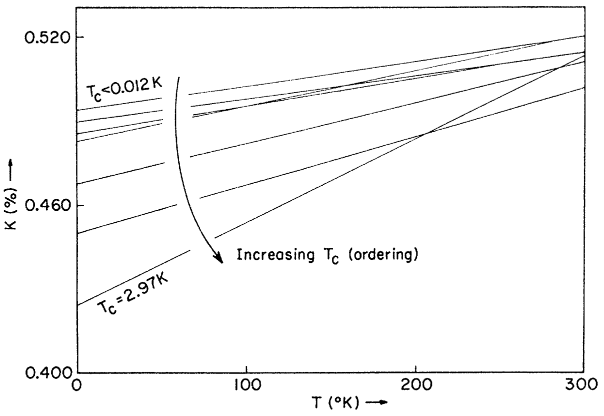

FIG. 1. The temperature-dependent Knight-shift variation in V_3Au with atomic ordering.

increase in $n(E)$, an exact explanation of this mechanism has not yet been shown.

We use as a basis the Labbé-Friedel[7] (LF) model which appears applicable for the ordered β-W structure in general.[8] In the LF model the tight-binding approximation (TBA) is used along the tightly packed orthogonal V-ion chains. We then introduce a small degree of disorder along the V chains in V_3Au by the substitution of Au ions into V positions. (Although it is more glamorous to speak of increasing T_c by ordering, our model is easier to present from the viewpoint of decreasing T_c by disordering.)

We first investigate the case of a finite-length V chain bounded by Au ions on its ends. There are n vanadium ions between the Au ions and we designate the ion-site position by v ($v=0$ at one Au ion, $v=n+1$ at the other end of the chain). There are then n electronic states in this chain, whose Bloch wave functions are of the type

$$\varphi_k(r)=\sum_{v=1}^{n}\Psi(\vec{r}-\vec{v}a)\sin kva, \tag{1}$$

where a is the distance between vanadium ions and $\Psi(\vec{r}-\vec{v}a)$ is the wave function of the atomic d orbital centered on the site v. Since Au is a nontransition element, we assume that the d-wave functions are pinned at the end of the chain, i.e., $\varphi(r)=0$ at $v=0$ and at $v=n+1$. Substituting these boundary conditions into (1) we see that

$$\sin k(n+1)a=0. \tag{2}$$

From (2), k can take the values

$$k=p\pi/(n+1)a, \tag{3}$$

where p is an integer from 1 to n corresponding to the n distinct electronic states [when $p=0$ or $n+1$, $\varphi_k(\vec{v})=0$]. We note that the value $p=n+2$ gives the same energy state as $p=n$ or more generally, the value for $p=n+1+s$ equals that for $p=n+1-s$.

We now investigate the electronic states associated with a very long V chain which is randomly interrupted by Au ions of concentration c. If there are N sites on this chain where N is very large, Nc of these sites will be occupied by Au ions and $N(1-c)$ will be occupied by V ions. We assume that $c\ll 1$ and that the Au-ion substitution is random along the chain. This will segment the long chain into many short chains of different lengths. Thus, we can define only an average chain length a/c which is the electronic mean free path.

For the entire chain of N ions, we define $g(k)$ as the number of electronic states whose wave numbers lie in the range from 0 to k. The density of states is then

$$n(k)=dg(k)/dk; \tag{4}$$

for any short chain of n vanadium ions, bounded by Au ions, the number of electronic states between 0 and k can be defined by $g_n(k)$. If f_n is the number of short chains containing n vanadium ions, then

$$g(k)=\sum_{n=n_k}^{N(1-c)} f_n g_n(k). \tag{5}$$

For a given value of k, the smallest n_k of n which contributes to $g(k)$ is defined by $\pi/(n_k+1)a<k\leqslant\pi/n_k a$. This in turn could be expressed as $n_k+1>\pi/ka\geqslant n_k$. The double inequality thus defines n_k as the integer part of π/ka. We see that we are investigating the values between 0 and π/a (but excluding these extremities) which occur at discrete intervals of $\pi/(n+1)a$. Thus, for a given value of k, the number of states in the range of 0 to k is simply the integer part of the ratio $k[\pi/(n+1)a]^{-1}$, or

$$g_n(k)=\{(n+1)ka/\pi\}, \tag{6}$$

where the curly brackets define an integer value only. In the case where $c\ll 1$, the average value of the number of v ions n between two Au ions is $1/c$ and therefore large. Since the integer value of a large quantity is approximately that quantity,

$$g_n(k)\simeq(n+1)ka/\pi. \tag{7}$$

We now seek the statistical distribution which will define f_n, the number of chains containing n vanadium ions. If we assume a Au ion to be located at the site $v=0$, we look for the probability of the occurrence of a short chain of n vanadium ions with Au ions at its extremities. The probability of having V ions at sites $v=1, v=2, \cdots, v=n$ is $1-c$ for each site. Similarly, the probability of Au ion being at the site $v=n+1$ is simply c. Thus, the probability of having a short chain of n vanadium ions is $(1-c)^n c$ where the probability is normalized to unity for $N \to \infty$. Since there are Nc gold ions along the quasi-infinite chain, this chain will be segmented into Nc short chains (including those chains for which $n=0$, where the nearest neighbors are Au ions). Thus, the number of short chains containing n vanadium ions between two Au ions is

$$f_n = Nc^2(1-c)^n. \tag{8}$$

Combining Eq. (5), (7), and (8), we obtain

$$g(k) \simeq Nc^2 \frac{ka}{\pi} \sum_{n=n_k}^{N(1-c)} (n+1)(1-c)^n, \tag{9}$$

which is calculated in the limit for N infinite and with $n_k = \{\pi/ka\}$. We get as a solution to (9)

$$g(k) = N(ka/\pi)(1+cn_k)(1-c)^{n_k}, \tag{10}$$

where $n_k = \{\pi/ka\}$.

We now introduce a function $g^{(0)}(k) = Nka/\pi$ which defines the number of states lying between 0 and k for an unperturbed chain with N sites, including no Au ions at all. Additionally, we can rewrite the last expression in Eq. (10) as

$$(1-c)^{n_k} = \exp[n_k \ln(1-c)].$$

For small concentration $c \ll 1$, $\ln(1-c) \simeq -c$, or $(1-c)^{n_k} \simeq \exp(-cn_k)$. Substitution into Eq. (10) leads to the final expression,

$$g(k) \simeq g^{(0)}(k)(1+cn_k)\exp(-cn_k) \tag{11}$$

with $n_k = \pi/ka$. Assuming the d sub-band to be symmetric about its center $k=\pi/2a$, we consider only the region $0 \leqslant k \leqslant \pi/2a$.

When we are far from the bottom ($k=0$) of the d sub-band, the quantity π/ka, and thus its integer part n_k, is not large. In this region $cn_k \ll 1$ is always realized. On expanding the exponential in (11), we see that the term of the first order in cn_k vanishes to give us

$$g(k) \simeq g^{(0)}(k)(1-\tfrac{1}{2}c^2 n_k^{\,2}). \tag{12}$$

This expression shows that far from the limits of the d sub-band, $g(k)$ is modified only by the second-order term for a small concentration c. Near the bottom ($k=0$) of the d sub-band, $k \ll \pi/a$ and $n_k \simeq \pi/ka$. Here Eq. (11) can be rewritten as

$$g(k) \simeq g^{(0)}(k)(1+c\pi/ka)\exp(-c\pi/ka). \tag{13}$$

If we take the derivative of Eq. (13) with respect to k we have an expression for the perturbed density of states $n(k)$ in k space:

$$n(k) \simeq n^{(0)}(k)\left\{1+\frac{c\pi}{ka}+\frac{c^2\pi^2}{k^2a^2}\right\}\exp\left(\frac{-c\pi}{ka}\right), \tag{14}$$

where $n^{(0)}(k) = (d/dk)g^{(0)}(k) = Na/\pi$ is the density of states for the unperturbed chain with N sites, including the case where there are no Au ions on the chain.

The density of states $n(E)$ as a function of energy E is given by $n(E) = n(k)dk/dE$, where we use the dispersion relation $E = E_0 - \frac{1}{2}W\cos ka$ of the unperturbed linear chain. (Although defects can lead to a suppression of states, the relation between E and k would remain unchanged.) We then find that

$$n(E) \simeq n^{(0)}(E)\left\{1+\frac{c\pi}{ka}+\frac{c^2\pi^2}{k^2a^2}\right\}\exp\left(\frac{-c\pi}{ka}\right), \tag{15}$$

where $n^{(0)}(E)$ is the unperturbed density of states.

In the above treatment, we see that a critical value of the wave number k appears at the value $c\pi/a$. We now consider the two extreme cases:

Case 1. For $c\pi/a \ll k \ll \pi/a$ we can expand the exponential in Eq. (15) to obtain

$$n(E) \simeq n^{(0)}(E)\left(1+\frac{1}{2}\frac{c^2\pi^2}{k^2a^2}\right). \tag{16}$$

Here the density of states is modified only by a term of the second order in the small concentration c of Au ions along the chain.

Case 2. For $k \ll c\pi/a$, we cannot expand the exponential in Eq. (15) since $c\pi/ka$ is much larger than unity. Thus, in this region, where k is very small (near the edge of the d sub-band), the density of states is decreased exponentially with the introduction of Au ions along the vanadium chains. Figure 2 shows both results schematically.

We have shown that in the region of a d sub-band near its edge where k is much less than $c\pi/a$, there is an enormous suppression of the density of states with the substitution of a small concentration of Au ions along the vanadium chains in the compound V_3Au. This appears to explain the experimental observation (R4) that the occupation of only 5% of the V sites by Au ions suppresses the core-polarization term of the total Knight shift. Additionally, the strong temperature dependence of the Knight shift of the ordered sample suggests a Fermi level lying close to the bottom of a d sub-band. Recent specific-heat data also show a strong reduction in the electronic specific heat due to small atomic disordering.[9] Such an effect is illustrated schematically in Fig.

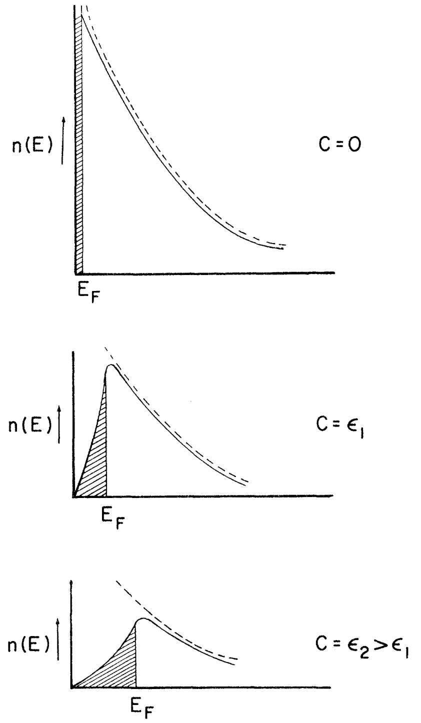

FIG. 2. Suppression of the density of states in V_3Au due to progressive degrees of disordering.

2, where a drastic suppression of $n(E)$ occurs with disordering.

In conclusion, there appears room for discussion on the mechanism for the drastic lowering of T_c with a small amount of disordering. It is still questionable whether this is directly due to a decrease in $n(E_F)$ or indirectly through the effect of $n(E_F)$ on the phonon spectrum. We suggest that further experimental data be obtained to clarify the mechanism. For example, one could measure the effects of small disorder on the phonon frequencies in V_3Au at low temperatures with neutron inelastic-scattering experiments. It would also be interesting, though less informative, to measure the effect of small disordering on the ultrasonic velocities at low temperatures.

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LUMINESCENCE FROM POLARITONS

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The intrinsic emission of CdS is studied at 20°K. We report the first clear-cut evidence of exciton polariton luminescence.

In 1958, Hopfield[1] predicted the existence of polaritons in crystals where there is strong coupling between direct excitons and photons. From absorption data Thomas and Hopfield[2-4] put into evidence a "longitudinal exciton" which can present a coupling with the electromagnetic field strongly dependent on the orientation of the wave vector of the absorbed photon. Observation of luminescence from this "longitudinal exciton" in uniaxial CdS has been reported previously[5-7] but no crucial experiments have been made to identify the origin of the observed polariton line.