

penstance, the deviation of T_S^* from T in the sphere of single crystal⁴ below 6 mdeg does not occur in the powder.

Finally, it is concluded that either Fermi-liquid theory does not agree with experiment, or the thermal and magnetic behavior of powdered CMN is anomalous. By anomalous is meant that the specific heat of powder does not go as $1/T^2$,¹⁰ whereas it goes as $1/T^2$ for a single crystal; furthermore, the interactions which cause T_S^* to deviate from T below 6 mdeg average to zero for particles as large as 1.4 mm. It is clear that for further progress in the field a clarification of the temperature scale is required; it is essential and urgently required to resolve the question raised here that magnetocaloric measurements, such as those made by Hudson and Kaeser⁵ on a single crystal, be made on a cylinder of powdered CMN.

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STATIC DIELECTRIC FUNCTION OF A ZERO-GAP SEMICONDUCTOR*

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In metals it is known that the static dielectric function $\epsilon(q)$ in the small q limit has a singularity. In the Fermi-Thomas (FT) approximation $\epsilon(q) = 1 + \lambda_{FT} T^2/q^2$, where the constant λ_{FT} is proportional to the density of states on the Fermi surface.¹ On the other hand, in an insulator $\epsilon(q) \rightarrow \epsilon_0$, the ordinary macroscopic dielectric constant.² This latter is a direct consequence of the energy gap in the one-particle electronic spectrum. In this paper we discuss a new type of screening intermediate between the above two cases. Specifically, we predict that in a certain special type of zero-gap semiconductor such as α -Sn, $\epsilon(q) \rightarrow \epsilon_0 \times [1 + \lambda/q]$ as $q \rightarrow 0$.

The expression for $\epsilon(q)$ in a solid in the frame-

work of the random phase approximation is given by^{3,4}

$$\epsilon(\vec{q}) = 1 - \frac{4\pi e^2}{q^2} \sum_{n, n', \vec{k}} |\langle \vec{k}, n | e^{-i\vec{q} \cdot \vec{r}} | \vec{k} + \vec{q}, n' \rangle|^2 \times \frac{N_{\vec{k} + \vec{q}, n'} - N_{\vec{k}, n}}{E_{\vec{k} + \vec{q}, n'} - E_{\vec{k}, n}}, \quad (1)$$

where n and n' are band index labels and $N_{\vec{k}, n}$ are occupation numbers. The matrix element just represents an overlap between the spatially periodic part of the two Bloch functions.

In α -Sn the conduction and valence bands make contact at the zone center and the degenerate band edge has Γ_8^+ symmetry.⁵ Therefore, the

structure of the $\vec{k}\cdot\vec{p}$ Hamiltonian is similar to that of the valence band edge of Ge. The difference is that in α -Sn, the light-hole band of Ge is inverted and becomes the conduction band. The energy spectrum sufficiently close to the zone center can be written as

$$E^c(\vec{k}) = \hbar^2 k^2 / 2m_c, \quad E^v(\vec{k}) = \hbar^2 k^2 / 2m_v, \quad (2)$$

provided we neglect a warping term. Here c and v refer to the conduction and valence band. The structure of the appropriate $\vec{k}\cdot\vec{p}$ Hamiltonian can be found in the literature.⁶ By directly diagonalizing the appropriate 4×4 $\vec{k}\cdot\vec{p}$ matrix, we find an explicit representation for the wave functions near $k=0$ in terms of those at the zone center. The result for the matrix element in Eq. (1) is then calculated to be

$$|\langle k, v | e^{-i\vec{q}\cdot\vec{r}} | \vec{k} + \vec{q}, c \rangle|^2 = \frac{3}{4} \frac{q^2 \sin^2 \theta}{k^2 + q^2 + 2kq \cos \theta}, \quad (3)$$

where θ is the polar angle between \vec{k} and \vec{q} , and \vec{q} for convenience is chosen along the (0, 1) axis.

In the two-band approximation we then find after direct integration of Eq. (1) that

$$\epsilon(q) = \epsilon_0(1 + \lambda/q), \quad (4)$$

where

$$\epsilon_0 = 1 - \frac{8e^2}{\pi \hbar^2 K} \frac{m_c m_v}{m_c + m_v} \quad (5)$$

and

$$\lambda = \frac{3e^2 m_v}{\hbar^2 \epsilon_0} \left[\frac{\pi}{2} - \left(\frac{m_v - m_c}{m_v} \right) \times \sin^{-1} \left(\frac{m_v}{m_v + m_c} \right)^{1/2} - \left(\frac{m_c}{m_v} \right)^{1/2} \right]. \quad (6)$$

K_m is chosen to give an integration volume equal to the Brillouin-zone size. Using the density-of-states effective masses for α -Sn, $m_c = 0.024m_e$ ⁷ and $m_v = 0.26m_e$,⁸ we get $\epsilon_0 = 0.88$ and $\lambda = 0.18 \text{ \AA}^{-1}$. Of course, in the evaluation of ϵ_0 , the coupling of states away from the zone edge and other bands is most important and this can be estimated to make $\epsilon_0 \approx 24$.⁹ This additional static screening causes us to modify λ to be ≈ 0.0066 .

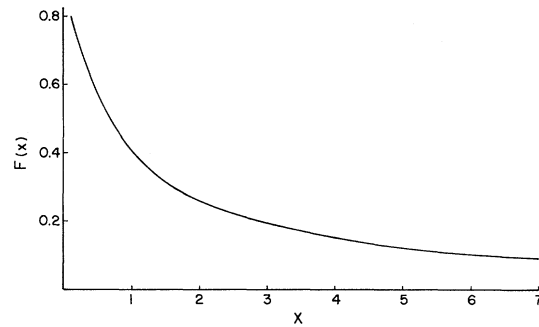


FIG. 1. The impurity potential is modified from the Coulomb behavior. The modulation function $F(x)$ is shown here.

This peculiar screening effect should make itself manifest through an enhanced free-carrier mobility when ionized-impurity scattering effects are the dominant mechanism. Some results of Lavine and Ewald¹⁰ indicate that such a mobility enhancement does take place in the low-concentration limit where a deviation from the expected concentration-independent value is observed. We also have investigated the spatial dependence of the impurity potential, and found a modification from the Coulomb behavior typical of a normal semiconductor. The potential is given by $V(r) = e^2 F(\lambda r) / r \epsilon_0$. $F(x)$ is plotted in Fig. 1. Details of the present calculation will be published.

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ORIGIN OF SOLVENT KNIGHT SHIFTS IN ALLOYS

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Detailed consideration of the rigid-band model for alloys shows that it predicts the correct sign and magnitude for changes in Knight shifts on the addition of nonmagnetic impurities to such solvents as Ag and liquid Cu. We conclude that while oscillatory impurity screening is important to these changes, analyses invoking it alone are significantly deficient.

The Knight shifts K of metals such as Ag,¹ Pb,² and liquid Cu³ display distinct valence effects on the addition of nonmagnetic impurities. The changes in the Knight-shift values ΔK upon alloying are normally attributed to modification of the hyperfine interaction resulting from changes in the behavior of the conduction electrons at the Fermi surface (these electrons screen the impurity charges^{4,5} via the Friedel oscillations). The ΔK are often assumed to arise entirely from this source.⁶ In practice, various pseudopotential and semiempirical phase-shift estimates of this have met with varying semiquantitative success.⁷ In this Letter, we show that an alternative scheme, the rigid-band model,⁸ also includes valence effects and yields ΔK behavior of the sign and magnitude observed experimentally. The incorrect behavior (i.e., ΔK of the opposite sign), which has been attributed to this model by some workers and cited as evidence for oscillatory impurity screening effects, is shown to be in error due to an inadequate assessment of the model. In particular, the variation with alloy-

ing in the hyperfine interaction of a conduction electron was omitted. From our results we conclude that, while the commonly invoked impurity screening effect may be important to ΔK , analyses employing it alone are significantly incomplete.

Let us consider the "rigid-band" model which is frequently invoked when considering many other properties of alloys.⁸ The addition of charge impurities of different valency than the host changes the number of conduction electrons per atom, n_e , and this shifts the Fermi level. For "free-electron" bands we have the Fermi wave vector given by $k_F = (3\pi^2 n_e / V)^{1/3}$, where V is the atomic volume in the alloy. When evaluating the Fermi contact interaction for such bands, it has been common to assume that the conduction electrons can be approximated by plane waves. However, the Pauli principle (expressed in the antisymmetry of the many-electron system) requires orthogonalization of the conduction-electron wave functions to those of the metal ion cores. Following this procedure, one obtains the Fermi-electron contact density

$$P_{\mathbf{F}} = |\varphi_{k_{\mathbf{F}}}(0)|^2 = [1 - \sum_{n,0} S_{n,0}^k k_{\mathbf{F}} R_{n,0}(0)]^2 \{V - 4\pi \sum_{n,l} (2l+1) (S_{n,l}^k k_{\mathbf{F}})^2\}^{-1}, \quad (1)$$