PHYSICAL REVIEW B VOLUME 31, NUMBER 1 1 JANUARY 1985

Comments

Comments are short papers which comment on papers of other authors previously published in the **Physical Review**. *Each Comment should state clearly to which paper it refers and must be accompanied by a brief abstract. The same publication schedule as for regular articles is followed, and page proofs are sent to authors.*

T_c degradation in disordered *A* 15 compounds

H. Gutfreund, M. Weger, and O. Entin-Wohlman*
Racah Institute of Physics, Hebrew University, Jerusalem 91904, Israel
(Received 9 December 1983)

Recently it was proposed by Anderson, Muttalib, and Ramakrishnan that the decrease of T_c with disorder in *A* 15 compounds can be attributed to an enhancement of the effective Coulomb repulsion, resulting from localization. We propose that the enhanced Coulomb repulsion can also be related to the quasi-one-dimensional nature of the *A* 15 compounds.

It has been known for some time that the transition temperature T_c of high-T_c *A* 15 compounds like V_3Si, Nb_3Ge, and similar materials is unusually sensitive to disorder, and that the depression of T_c can be correlated in a "universal" manner with the resistivity, regardless of what caused the disorder.[1] In a recent publication Anderson, Muttalib, and Ramakrishnan[2] (to be referred as AMR) have attributed this depression to an increase in the Coulomb pseudopotential μ^* in a strongly disordered system. Their argument concerns the scale size dependence of the diffusion associated with the onset of Anderson localization. The charge-density fluctuations diffuse more slowly over a scale size which increases with disorder and therefore interact more strongly, leading to an increase in μ^*. The starting point of AMR is the expression for the Coulomb kernel in the strong-disordered regime

$$K^c(\omega) = \mu + 2V_S \int dt\, P(t)\cos(\omega t) \ , \tag{1}$$

where V_S is the local screened Coulomb potential, μ is the interaction parameter, $\mu = N(\epsilon_F)V_S$, where $N(\epsilon_F)$ is the density of states. In (1), $P(t)$ is the diffusional autocorrelation function between charge fluctuations, that is, it is the probability that an electron has not diffused away in a time t. It changes from the classical $t^{-3/2}$ behavior to a slower t^{-1} decrease as one crosses to the localization region where the diffusion is nonclassical. The reduced diffusion over a length scale which increases with increasing disorder results in a retarded and enhanced Coulomb repulsion. However, AMR find that the critical resistivity at which localization occurs in a free-electron gas is much higher (by a factor of 25) than the resistivities required to interpret the experimental T_c vs ρ dependence. This discrepancy is attributed to various factors.

In the present Comment we wish to point out a different possible cause for a reduced decay of the charge-density fluctuations. AMR do not consider the anisotropic nature of the *A* 15 compounds related to the linear-chain structure of the transition-metal atoms.[3] We propose that the one-dimensional (1D) character of diffusion along the chains plays a key role and leads to an increase in μ^* which is correlated with the right order of magnitude of the resistivity. We first exhibit this, and then summarize the evidence for the quasi-one-dimensionality.

In order to use Eq. (1) we need a form for the autocorrelation function $P(t)$. In a pure 1D system $P(t)$ is given by $(4\pi Dt)^{-1/2}$, where D is the diffusion constant along the chains. When this expression is inserted into Eq. (1), the time integral diverges. In real systems this divergence is suppressed by the fact that electrons escape from one chain to another after a characteristic time[4] $\tau_\perp$. Thus in our model

$$P(t) = \frac{1}{(4\pi Dt)^{1/2}} e^{-t/\tau_\perp} \ . \tag{2}$$

We now assume that the diffusion along the chains is classical and obtain

$$\int_0^\infty dt\, P(t)\cos(\omega t) = \sqrt{\tau_\perp/8D}\, \frac{\{[(\omega\tau_\perp)^2+1]^{1/2}+1\}^{1/2}}{[(\omega\tau_\perp)^2+1]^{1/2}} \ . \tag{3}$$

In[3,5] V_3Si $\omega_D\tau_\perp < 0.3$, where ω_D is the Debye frequency, so that Eq. (3) is independent of ω at $\omega \lesssim \omega_D$ and decreases with ω at high frequencies. To get a quantitative estimate of the effect we take the $(\omega\tau_\perp)^2 << 1$ limit and find

$$K^c = \mu + \frac{V_S}{\hbar v_F S}\frac{\overline{\tau}_\perp}{\tau_\parallel} \ . \tag{4}$$

Here we have used the free-electron expression for the diffusion constant, $D = v_F^2\tau_\parallel$, where $\tau_\parallel$ is the backscattering time along the chains, and S is the cross section of the unit cell perpendicular to the chains.

Finally, we point out that $\tau_\perp$, the tunneling time between chains, is generally related to $\tau_\parallel$. In a coupled chain system[6]

$$\frac{\hbar}{\tau_\perp} = \frac{t_\perp^2\tau_\parallel}{\hbar} \ , \tag{5}$$

where $t_\perp$ is the transfer integral between chains. This expression for the transition probability between chains is the analog of the "golden rule." It shows that a decrease in $\tau_\parallel$ enhances the lifetime on a chain-intrachain scattering and interferes with interchain tunneling. In *A* 15 compounds the situation is more complicated. Here the transfer integrals $t_\perp$ between individual atoms on two perpendicular chains are rather large, but the one-dimensional character follows in part from a cancellation effect due to destructive interference, for example, between the overlap of the lobes of an atomic wave function on one chain with the lobes of wave functions on two atoms on a perpendicular chain[3] or between π-π and π-σ scattering.[7] This results in a small effective $t_\perp$. When the electron mean free path l on a chain is of the order of the atomic spacing this destructive interference is violated and for very short $\tau_\parallel$, $\tau_\perp$ decreases together with $\tau_\parallel$. However, as long as $k_F l > 2$, we expect Eq. (5) to be valid. The condition $k_F l > 2$ is essential for the validity of our model. When $k_F l \simeq 1$, $P(t)$ goes like t^{-1} even in one dimension so that in the critical region (of the Anderson localization) the argument of AMR is independent of dimension. It is hard to evaluate $k_F l$ up to a factor of 2, but one can get an order of magnitude estimate from the relation $\sigma = ne^2 l/P_F$. The main question is the value of n—the density of electrons contributing to the conductivity. From the comparison of the size of the Fermi surface to the size of the first Brillouin zone[3,8] we calculate that there are approximately 2–3 conduction electrons per unit cell. The other bands are full. Taking $n = 2.5$, $k_F = \pi/2a$, where a is the lattice constant,[3,8] we find for $\rho = 100\ \mu\Omega\,\text{cm}$ that $k_F l \simeq 2$. Thus in the entire range in question ($\rho = 20$–$100\ \mu\Omega\,\text{cm}$) $k_F l \simeq 2$. Using Eq. (5) in Eq. (4),

$$\mu' = \mu + \Delta\mu = \mu + \alpha \frac{\hbar}{t_\perp \tau_\parallel} \ , \tag{6}$$

where $\alpha = V_S/\hbar v_F S$.

We shall now check if this expression can account for the right order of magnitude of the depression of T_c with ρ, assuming that $\rho \propto \tau_\parallel^{-1}$. We use McMillan's formula

$$T_c = \frac{\omega_d}{1.45} \exp\left[-\frac{1.04(1+\lambda)}{\lambda - \mu^*(1+0.62\lambda)} \right] \ , \tag{7}$$

where

$$\mu^* = \frac{\mu'}{1 + \mu' \ln(\epsilon_F/\omega_D)} \ . \tag{8}$$

Like AMR we neglect the effect of disorder upon the phonon-induced attraction λ, and take for V_3Si $\lambda = 1.2$, $\omega_D = 330$ K, and $\mu = 0.3$. We estimate that $\ln(\epsilon_F/\omega_D) \simeq 2$ for the following reason: ϵ_F is approximately the half-width of the peak in the density of states. This peak was measured by Fradin and Zamir[5] in V_3Ga and similar alloys, and was found to be about 0.4 eV wide. The calculations of Van Kessel and co-workers[5] for Nb_3Sn show a peak of this width. This peak is largely due to the π band. There are narrower peaks, due to the δ bands, but we feel that they do not contribute much to T_c.[5] Thus, taking $\epsilon_F \simeq 0.2$ eV and $\omega_D = 330$ K yields $\ln(\epsilon_F/\omega_D) \simeq 2$. With these values we find that when T_c changes from 14 to 5 K, $\Delta\mu$ in Eq. (6) has to increase by a factor of 10 (from 0.09 to 0.8). In this range the resistivity changes by a factor of 5 (from $\rho = 20$–$100\ \mu\Omega\,\text{cm}$). It is needless to say that we can hardly expect a better agreement from such crude estimates. Let us now check the numerical value of $\Delta\mu$. V_S is the Coulomb potential due to the electrons in the peak of the density of states screened by all the electrons. Hence α is given approximately by

$$\alpha = \frac{1}{N(\epsilon_F)} \frac{1}{S} \frac{1}{\hbar v_F} \ , \tag{9}$$

where $N(\epsilon_F)$ is the 3D density of states. Therefore α gives the ratio of conduction electrons contained in the peak of the density of states to the total number of the conduction electrons. Since the peak (of width of the order 0.4 eV) contains about 10% of the conduction electrons,[3] we estimate $\alpha \simeq 0.1$. Reasonable estimates of $t_\perp$ and $\tau_\parallel$ are $t_\perp \simeq 0.1$ eV (Ref. 5) and $\hbar/\tau_\parallel$ of the order 0.2–0.4 eV (corresponding to a mean free path of several atomic distances). Thus an order of magnitude estimate of $\Delta\mu$ is in accordance with reasonable values of $t_\perp$ and $\tau_\parallel$.

In the remaining part of this Comment we summarize the theoretical and experimental evidence for the quasi-one-dimensional nature of the $A15$ compounds.

The quasi-one-dimensional character of the band structure is caused by several factors:[3] (i) for the σ and π bands, the lobes of the wave functions point along the chains, and therefore the interchain transfer integrals are smaller than the intrachain ones; (ii) for certain states, in certain regions of the Brillouin zone, there is a destructive interference effect between interchain scattering from neighboring atoms, or from different orbitals; (iii) since the chains in close contact are orthogonal, a given interchain transfer integral has a smaller effect in destroying the "one-dimensionality" than a similar integral between parallel chains.

The theoretical calculations of the electronic band structure[3,5,8] indicate that the linear-chain structure gives rise to planar sections of the Fermi surface. The destructive interference effect occurs only in certain regions of the Brillouin zone, and therefore the planar sections do not extend over the whole zone.

Experimentally, the anisotropic nature manifests itself in a number of ways. (i) A very anisotropic depression of T_c is due to uniaxial stress in the (100) direction, in V_3Si and Nb_3Sn. Stress in the (111) direction does not have any significant effect, and hydrostatic pressure actually raises T_c of V_3Si.[9] (ii) Tunneling experiments[10] into a single crystal of Nb_3Sn indicate a gap corresponding to $T_c = 15$ K for a surface in the (100) plane, $T_c = 11$ K for a surface in the (110) plane, and $T_c = 5$ K for a surface in the (111) plane. (iii) Positron annihilation experiments[8,11] indicate peaks in the derivative of the momentum distribution in the (100) direction. (iv) In Nb_3Al the NMR relaxation rate is enhanced well above T_c, suggesting one-dimensional fluctuations.[12]

We agree with AMR that it is unrealistic to explain the strong depression of T_c with ρ by the smearing of the peaks in the density of states with increasing disorder. The electronic density of states possesses sharp peaks which are smeared by disorder, but these are not present in all high-T_c $A15$ compounds, for example, not in Nb_3Al and thus seem not to be essential for the high value of T_c. This point is also emphasized by AMR who refer to tunneling data[13] to support it. There is also a somewhat broader peak near ϵ_F, but it arises from a rather large region in the Brillouin zone,[5,7] and therefore we do not expect disorder to have a drastic effect on it (unless the disorder is very large and the material is essentially amorphous). A different mechanism for the degradation of T_c was proposed by Ruvalds and

Soukoulis.[14] It is based on the assumption that acoustic plasmons play a dominant role in the superconductivity of $A15$ compounds and on an investigation of the effect of disorder on acoustic plasmons. The problem with this interpretation is that there is so far no empirical evidence for the existence of acoustic plasmons in $A15$ compounds.

Our conclusion is that the strong depression of T_c can be related to the effect of disorder on μ^*. Taking into account the quasi-one-dimensional nature of the $A15$ compounds, we have found that the increase in μ^* is in agreement with the depression of T_c with ρ data.

ACKNOWLEDGMENTS

We are grateful for helpful discussions with J. Appel. This research was supported by a grant from the National Council for Research and Development, Israel, and the Kernforschungszentrum Karlsruhe, Karlsruhe, Germany.

---

[*] Permanent address: Department of Physics and Astronomy, Tel Aviv University, Tel Aviv 69978, Israel.

[1] L. R. Testardi, J. M. Poate, and H. J. L. Levinstein, Phys. Rev. B **15**, 2570 (1977); A. K. Ghosh, H. Weissman, M. Gurevitch, H. Lutz, O. F. Kammerer, C. L. Snead, A. Goland, and M. Strongin, J. Nucl. Mater. **72**, 70 (1978); A. R. Sweedler, D. E. Cox, and S. Moechlecke, *ibid.* **72**, 50 (1978).

[2] P. W. Anderson, K. A. Muttalib, and T. V. Ramakrishnan, Phys. Rev. B **28**, 117 (1983).

[3] M. Weger and I. B. Goldberg, in *Solid State Physics: Advances in Research and Applications, Vol. 28,* edited by D. Turnbull, F. Seitz, and H. Ehrenreich (Academic, New York, 1973), p. 1; M. Weger, J. Less-Common Met. **62**, 39 (1978).

[4] G. Soda, D. Jerome, M. Weger, J. M. Fabre, and L. Giral, Solid State Commun. **18**, 1417 (1976).

[5] A. T. Van Kessel, H. W. Myron, and F. M. Mueller, Phys. Rev. Lett. **41**, 181 (1978); F. Y. Fradin and D. Zamir, Phys. Rev. B **7**, 4861 (1978); O. Entin-Wohlman and M. Weger, Synth. Met. **5**, 217 (1983).

[6] M. Weger, J. Phys. (Paris) Colloq. **39**, C6-1456 (1978).

[7] L. F. Mattheiss and W. Weber, Phys. Rev. B **25**, 2248 (1982).

[8] T. Jarlborg, A. A. Manual, and M. Peter, Phys. Rev. B **27**, 4210 (1983).

[9] M. Weger, B. G. Silbernagel, and E. S. Greiner, Phys. Rev. Lett. **13**, 521 (1964).

[10] V. Hoffstein and R. W. Cohen, Phys. Lett. **29A**, 603 (1969) M. Weger, Solid State Commun. **9**, 107 (1971).

[11] S. Samuelov, M. Weger, I. Nowik, I. B. Goldberg, and J. Ashenazi, J. Phys. F **11**, 1281 (1981); S. Berko and M. Weger, Phys. Rev. Lett. **24**, 55 (1970).

[12] T. Maniv, Solid State Commun. **26**, 115 (1978).

[13] J. Kwo, T. P. Orlando, and M. R. Beasley, Phys. Rev. B **24**, 2506 (1981).

[14] J. Ruvalds and C. M. Soukoulis, Phys. Rev. Lett. **43**, 1263 (1979).