Dephasing rate in metals versus diffusion constant

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We discuss correlation between the dephasing time for weak localization in three-dimensional (3D) metals and their conductance. Such correlation was reported for 3D In_2O_{3-x} films [Z. Ovadyahu, Phys. Rev. Lett. **52** 569 (1984)] and recently in several 3D alloys [J.J. Lin and L.Y. Kao, J. Phys.: Condens. Matter **13**, L119 (2001)]. We show that the observed correlation can be explained by the model based on tunneling states of dynamic structural defects.

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As early as in 1984, in the course of a study of weak localization corrections to the conductivity of three-dimensional (3D) In_2O_{3-x} films, Ovadyahu[1] observed a puzzling behavior of the electron dephasing time τ_φ as a function of static disorder. Namely, for a given temperature the dephasing rate τ_φ^{-1} scaled with the sample conductivity. This contradicted naive expectations that disorder should lead to an increase of the scattering rate. At first sight, such a behavior could have been ascribed to the disorder-mediated electron-phonon scattering proposed by Schmid[2] for dirty metals. However, such a mechanism must have been ruled out because of the observed temperature dependence of $\tau_\varphi \propto 1/T$ (at temperatures $\gtrsim 10$ K),[1] and to the best of our knowledge this scaling has waited to be explained ever since.

There has been a recent resurrection of interest in the topic in connection with the problem of the low-temperature behavior of the weak localization dephasing rate. This problem was extensively discussed during last years; see for a review Ref. 3 and references therein. In particular, an important correlation between the low-temperature dephasing rate and the diffusion constant D, $\tau_\varphi^{-1} \propto D$, was reported for several 3D polycrystalline disordered metals.[3,4]

In the present paper we demonstrate that this correlation finds its natural explanation within the framework of the model of the tunneling states (TS's) considered in Ref. 5. According to this model, dephasing is generated by dynamical structural defects that can assume two (or more) configurations with very close energies. Due to the interaction with a thermal bath, these defects switch between the states corresponding to these configurations producing time-dependent fields acting on electrons.

Two specific mechanisms of electron dephasing due to dynamic defects can be distinguished. The first mechanism is related to the direct inelastic transitions between the levels of the TS's. This implies a possibility for determining the actual path of the electron and, consequently, the loss of the interference. The second mechanism is due to the relaxational dynamics of TS's themselves, which fluctuate because of the interaction with the thermal bath. The emerging time dependence of the electron scattering crossection leads to violation of the time-reversal symmetry and, as a consequence, to decoherence. The effective Hamiltonian of a TS,

$$\tilde{\mathcal{H}}_d = (\Delta\sigma_3 - \Lambda\sigma_1)/2, \tag{1}$$

is characterized by the asymmetry Δ and the tunneling matrix element Λ. Here σ_1 and σ_3 are Pauli matrices. The physical meaning of the parameters Δ and Λ is clear from Fig. 1.

Since Δ and Λ are random, their distribution $\mathcal{P}(\Delta,\Lambda)$ is crucially important. In crystalline materials, it is natural to assume that the TS's keep intrinsic crystal symmetry. As a result, the Λ distribution is peaked about some value Λ_0. To keep the model simple it is sufficient to assume that $\mathcal{P}(\Delta,\Lambda) \propto \delta(\Lambda - \Lambda_0)$.

To evaluate the distribution over Δ let us assume[6] that the distribution is generated by some mesoscopic disorder around a generically symmetric defect and consider adiabatic renormalization of the site energy ε_1 of one of the TS components by conduction electrons scattering on the ith defect,[6]

$$\varepsilon_{1i} = V_1 \mathrm{Re}\left[\sum_{\mathbf{k}} \frac{f_i(\theta)}{R_{1i}} \frac{e^{ikR_{1i}(1-\cos\theta)}}{1+e^{(\varepsilon_{\mathbf{k}}-\varepsilon_F)/k_BT}}\right].$$

Here $\theta = \angle\{\mathbf{k},\mathbf{R}_{1i}\}$, f_i is the scattering amplitude by the ith defect, and $\mathbf{R}_{1j}$ is the vector connecting sites 1 and i (see

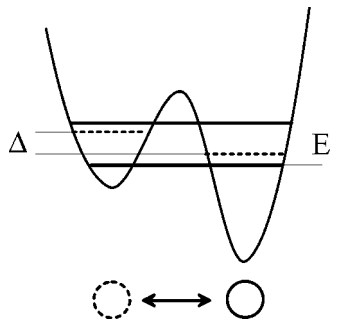

FIG. 1. Sketch of the effective potential describing a tunneling state (TS). The interlevel splitting E is determined by the diagonal asymmetry Δ and tunneling matrix element Λ as $E = \sqrt{\Delta^2 + \Lambda^2}$.

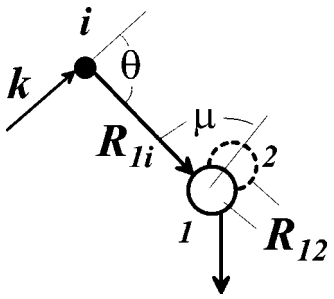

FIG. 2. Calculation of the adiabatic renormalization of the TS's diagonal splitting.

Fig. 2), while V_1 is the potential of defect 1. This correction comes from Friedel oscillations of the electron density induced by the ith defect.

Assuming that the scattering potentials for the defects 1 and i are the same we get an order-of-magnitude estimate for this quantity as

$$\varepsilon_{1i} \approx -\frac{|V|^2}{\varepsilon_F} \frac{\cos(2k_F R_{1i})}{(k_F R_{1i})^3}.$$

Now consider a TS formed by site 1 and some state 2, such that $R_{12} \ll R_{1i}, R_{2i}$. Then the effective two-level system acquires the diagonal splitting $\Delta_i \equiv (\varepsilon_{1i} - \varepsilon_2)$ given by the expression

$$\Delta(\mathbf{R}_i, \mu) \approx \frac{2|V|^2}{\varepsilon_F} \frac{\sin(k_F R_{12} \cos\mu)\sin(2k_F R_i)}{(k_F R_i)^3}. \quad (2)$$

Here $\mathbf{R}_i = \mathbf{R}_{1i} \approx \mathbf{R}_{2i}$, $\mu = \angle\{\mathbf{R}_{12}, \mathbf{R}_i\}$. The probability to find a TS with splitting Δ is then

$$W(\Delta) = 2\pi n_d \int R^2 dR \int_{-1}^{1} d(\cos\mu)\, \delta[\Delta - \Delta(\mathbf{R}, \mu)]. \quad (3)$$

Here n_d is the density of static defects, while $\Delta(\mathbf{R}, \mu)$ is given by Eq. (2). Hence the density of TS's is given by the expression $\mathcal{P}(\Delta) = N_{TS} W(\Delta)$ where N_{TS} is the density of TS's. Note that the main contribution to the integral in Eq. (3) comes from the distances $R \lesssim N_D^{-1/3}$: since the effects of different defects have quasirandom signs, the nearest defects appear most influential.

A straightforward analysis shows that there is a characteristic energy

$$E^* = \frac{|V|^2 n_d}{\varepsilon_F k_F^3} \approx \frac{1}{2\pi} \frac{\hbar}{\tau_{el}} \sim \frac{\hbar v_F^2}{D}, \quad (4)$$

where τ_{el} is the elastic mean free time, which separates different regimes of the $W(\Delta)$ behavior. At $\Delta \gg E^*$ the probability $W(\Delta)$ decays $\propto E^*/\Delta^2$, whereas at $\Delta \lesssim E^*$ the function $W(\Delta)$ is smooth. As a result, we arrive at the model for the density of TS's adopted in Ref. 5,

$$\mathcal{P}(\Delta, \Lambda) \approx (N_{TS}/E^*)\, \delta(\Lambda - \Lambda_0). \quad (5)$$

As shown in Ref. 5, the dephasing rate τ_φ^{-1} can be estimated in the relevant temperature region as

$$\tau_\varphi^{-1} = \tau_\Lambda^{-1}[\alpha(T\tau_\Lambda/\hbar)^{1/3} + \zeta]. \quad (6)$$

Here $\tau_\Lambda^{-1} = \nu_{TS}(\Lambda_0/E^*)$, ν_{TS} is the effective collision frequency with the tunneling defects, and α and ζ are constants of order 1. Since $\tau_\Lambda^{-1} \propto D$, we conclude that for a fixed number of tunneling defects the "saturated" dephasing rate *increases* with the diffusion constant D, and the corresponding dependence of τ_φ^{-1} tends to direct proportionality when the two items in Eq. (6) are comparable. Thus, Eq. (6) qualitatively explains both slow temperature dependence (apparent saturation) of the dephasing rate at low temperatures and its correlation with conductance. Such a combination has been observed in Refs. 3 and 4.

The above formulas should be viewed rather as order-of-magnitude estimates than quantitative results. Assuming a typical elastic relaxation time $\tau_{el} \approx (1-3) \times 10^{-14}$ s we obtain the values for E^* from a few dozens to 100 K. More detailed numerical estimates for the dephasing rate are given in Ref. 5. Those estimates are based on parameters extracted from experiments with point contacts and result in $\tau_\varphi \sim 10^{-9}$ s, which are of the same order of magnitude as those found in experiments.

Finally, we would like to emphasize that the discussed correlation between the dephasing rate and the conductance is rather insensitive to the details of the model for tunneling defects. Indeed, the above consideration is built on two assumptions: (i) the density of dynamic defects is fixed within the ensemble of samples and (ii) the density of states is proportional to $1/E^*$ where the dispersion in the defect energies E^* is controlled by disorder. Consequently, if these two requirements are met, then a correlation between τ_φ^{-1} and the diffusion constant D should exist for a wide class of distributions of the tunneling matrix element Λ. Here we return to the results obtained for three-dimensional low-resistivity In_2O_{3-x} films[1] where the observed temperature dependence of the dephasing rate was $\tau_\varphi^{-1} \propto T$. The samples showing such a behavior were rather disordered [$\tau_{el} \approx (2-5) \times 10^{-15}$ s]; the most probable origin for disorder was, probably, the oxygen nonstoichiometry. We conjecture that the mobile defects in In_2O_{3-x} films are created by the nonstoichiometric oxygen atoms. Then, for a given x, the number of atoms contributing to dynamics is expected to be fixed. At the same time, rather strong disorder can also affect the barriers for mobile defects, creating "soft" configurations such as in structural glasses. As a result, the distribution function of the tunneling matrix elements behaves as $\propto 1/\Lambda$, implying

a linear temperature dependence of the dephasing rate, $\tau^{-1} \propto T$. The spread E^* of the diagonal splittings Δ is probablystill determined by Friedel oscillations of the electron density keeping the dephasing rate proportional to the diffusion constant (or to the elastic mean free path). To conclude, we feel that the proposed model can well explain the experimental findings by Ovadyahu.[1]

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