Residual resistivity dipoles, electromigration, and electronic conduction in metallic microstructures

by R. S. Sorbello
C. S. Chu

For an impurity in a bulk metal, the connection between electromigration and electric fields associated with dc conductivity is understood in terms of Landauer's residual resistivity dipole. This connection is examined, and appropriate generalizations are made for an impurity in a two-dimensional electron gas and for an impurity near a metal surface. The residual resistivity dipole field decays less rapidly with distance in a two-dimensional gas than in bulk, thus resulting in a larger voltage drop across an impurity in the system of lower dimensionality.

1. Introduction

When a single impurity is introduced in bulk metal, the resistivity of the sample is increased. Conventional theories of electronic conduction ignore the spatial variation of the microscopic electric field and current in the vicinity of the impurity. Presumably, the justification for ignoring these microscopic spatial variations is that we are interested in macroscopic systems with random distributions of impurities. Microscopic spatial fluctuations are expected, on average, to cancel out. It thus appears reasonable to perform calculations based on the existence of a uniform electric field. The actual situation is more complicated and more interesting, and was elucidated by Landauer in his classic 1957 paper [1]. According to Landauer, the increased resistivity due to an impurity is associated with a microscopic dipolar source of electric field and current [1–3]. This is the residual resistivity dipole (RRD).

Analyses of electronic conduction based upon the RRD picture have not yielded new answers for the residual resistivity [1, 2]. However, if one is interested in the local field in the vicinity of an impurity, the RRD picture is essential. The local field acts as a driving force on an ion in a solid, and thus the RRD is conceptually important for an understanding of electromigration [4, 5], which is the phenomenon of atomic transport in the presence of electron current. In addition, it now appears possible to measure directly the voltage drop across a defect in a microstructure, thereby actually probing RRD fields [6]. The experiments have thus far probed local voltage drops across a single defect only in the weak-localization regime where quantum interference effects play an important role [7]. In general, we believe that knowledge of microscopic fields and currents is essential in the understanding of electron transport and electromigration in metallic microstructures. Here Landauer's approach provides crucial insight.

In this paper we extend the Landauer RRD picture to two cases of interest for metallic microstructures, namely to the case of an impurity in a two-dimensional electron gas, and to the case of an impurity near the surface of a metal. We first examine the case of an impurity in a bulk metal, where the usual Landauer analysis applies. In an effort to make some aspects of Landauer's theory more "user-friendly" to workers comfortable with more traditional methods, we describe a transport-equation method rather than the original Landauer method for evaluating the long-range RRD field. The transport equation method is, in fact, mentioned by Landauer [2].

2. Impurity in bulk metal

We consider a single impurity in a bulk metal sample characterized by a uniform background scattering time τ which gives rise to the usual bulk resistivity $\rho_0 = m/ne^2\tau$. The electrons have density n, mass m, and charge $-e$, and are considered in a jellium model. In the absence of the impurity, the electron distribution for a current-carrying sample is a shifted Fermi sphere. The part of the distribution which is linear in the uniform macroscopic electric field $\vec{E}_0$ is given by

$$g_{\vec{k}}^0 = -\tau e\vec{v}_{\vec{k}} \cdot \vec{E}_0 \delta(\epsilon_k - \epsilon_F), \tag{1}$$

where $\vec{v}_{\vec{k}} = \hbar\vec{k}/m$ is the electron velocity, ϵ_k is the electron energy $\hbar^2k^2/2m$, and ϵ_F is the Fermi energy. The electron charge current carried by $g_{\vec{k}}^0$ is given by $\vec{J}_0 = \vec{E}_0/\rho_0$.

An impurity is now placed in the electron gas. Consider the scattering taking place within a spherical region of radius r_0 centered at the impurity. Take $r_0 \ll \ell$, where $\ell = \hbar k_F\tau/m$ is the mean free path (k_F is the Fermi wavevector). The electron scattering states $\psi_{\vec{k}}$ have the asymptotic ($k_F r \gg 1$) form

$$\psi_{\vec{k}}(\vec{r}) \sim \frac{1}{\Omega^{1/2}}\left[e^{i\vec{k}\cdot\vec{r}} + \frac{f(\theta)}{r}e^{ikr}\right], \tag{2}$$

where $f(\theta)$ is the scattering amplitude and Ω is the crystal volume. The corresponding electron density due to the electron current, or "electron wind," is [3, 8]

$$\delta n_w(\vec{r}) = \sum_{\vec{k}} g_{\vec{k}}^0 |\psi_{\vec{k}}(\vec{r})|^2. \tag{3}$$

The electrostatic potential, $\delta\Phi(\vec{r})$, arises from $\delta n_w(\vec{r})$ and the induced screening charge, $\delta n_s(\vec{r})$, which attempts to locally neutralize $\delta n_w(\vec{r})$. Within a Thomas–Fermi approximation, self-consistent screening gives [1, 3]

$$\delta\Phi(\vec{r}) = -\frac{1}{e}(dn/dE)^{-1}\delta n_w(\vec{r}), \tag{4}$$

where dn/dE is the electron density of states at the Fermi level.

It is straightforward to evaluate $\delta\Phi$ in the asymptotic region using Equations (1)–(4). The result is the RRD potential

$$\delta\Phi(\vec{r}) = -\frac{p\cos\theta}{r^2}, \tag{5}$$

where $\cos\theta = \hat{r}\cdot\hat{E}_0$ and the dipole moment p is given by

$$p = \frac{3\pi\hbar I_0 S_0}{4k_F^2 e}. \tag{6}$$

Here I_0 is the particle current density far from the impurity ($I_0 = |\vec{J}_0|/e$), and S_0 is the scattering transport cross section given by

$$S_0 = \int |f(\theta)|^2(1 - \cos\theta)d\Omega. \tag{7}$$

Expressions (5) and (6) apply in the quantum-mechanical asymptotic regime $\ell \gg r \gg k_F^{-1}$.

The electromigration wind force equals the momentum transfer per second to the impurity due to collisions with the electrons. We can determine this from the asymptotic form of the radial current density J_r. The wind force, F_w, becomes

$$F_w = \hbar k_F \int J_r(\vec{r})\hat{r}\cdot\hat{E}_0 r^2 d\Omega_{\hat{r}}, \tag{8}$$

where

$$J_r(\vec{r}) = \sum_{\vec{k}} g_{\vec{k}}^0 \frac{\hbar}{m}\left[\mathrm{Re}\left\{\frac{1}{i}\psi_{\vec{k}}^*(\vec{r})\frac{\partial}{\partial r}\psi_{\vec{k}}(\vec{r})\right\} - \frac{\vec{k}\cdot\hat{r}}{\Omega}\right]. \tag{9}$$

A positive value of F_w indicates a force in the direction opposite to $\vec{E}_0$, i.e., along the direction of the electron wind. In using Equations (8) and (9), we are to take the asymptotic form (2). The result is

$$F_w = \frac{4k_F^3 e}{3\pi}p. \tag{10}$$

When r is of the order of ℓ or greater, the RRD field can be found by solving the transport equation, with the current J_r acting as a point source [2]. The dynamic electron distribution $g_{\vec{k}}$ satisfies the transport equation

$$\vec{v}_{\vec{k}}\cdot\vec{\nabla}_r g_{\vec{k}} + \vec{v}_{\vec{k}}\cdot e\vec{E}_0\delta(\epsilon_k - \epsilon_F) = -\frac{(g_{\vec{k}} - \bar{g}_{\vec{k}})}{\tau} + S_{\vec{k}}(\vec{r}), \tag{11}$$

where $\bar{g}_{\vec{k}} = (1/4\pi)\int d\Omega_{\hat{k}} g_{\vec{k}}$ is the local average to which the electrons relax. The source term has the form

$$S_{\vec{k}}(\vec{r}) = \delta(\vec{r})\delta(\epsilon_k - \epsilon_F)s(\hat{k}) \tag{12}$$

with

$$s(\hat{k}) = \frac{4\pi^3\hbar^2}{mk_F}J_r(\vec{r})r^2\Big|_{\hat{r}=\hat{k}}. \tag{13}$$

The source term is contrived so that it corresponds to a particle current $J_r(\vec{r})$ emitted from the scatterer.

The solution of Equation (11) is facilitated by the substitution

$$g_{\vec{k}} = g_{\vec{k}}^0 + G(\hat{k}, \vec{r})\delta(\epsilon_k - \epsilon_F)$$

and subsequent Fourier transformation taking $\exp(i\vec{q}\cdot\vec{r})$ spatial variation. After some algebra one obtains an expression for $G(\hat{k}, \vec{q})$ which can be Fourier-transformed analytically to obtain $G(\hat{k}, \vec{r})$. The resulting electron density $\delta n_w(\vec{r})$ follows upon performing the sum of $g_{\vec{k}}$ over $\vec{k}$. The result is

$$\delta n_w(\vec{r}) = \left(\frac{mk_F e}{\pi^2\hbar^2}\right)\frac{p\cos\theta}{r^2}. \tag{14}$$

Since the factor in parentheses equals edn/dE, we deduce from Equations (4) and (14) that $\delta\Phi(\vec{r})$ is given by the expression (5). Thus, the RRD retains its dipolar field pattern in the presence of background scattering, i.e., when r is comparable to, or greater than, ℓ. We emphasize, along with Landauer [1, 2], that $\delta\Phi(\vec{r})$ effects are properly accounted for via Equation (4). $\delta\Phi(\vec{r})$ should *not* be placed as a driving field in the Boltzmann equation (11).

Consider the resistivity change, $\delta\rho$, for an impurity between two large, parallel mathematical surfaces of area A separated by a distance L_x, where $L_x \ll A^{1/2}$. The average of $\delta\Phi$ over one surface has magnitude $2\pi p/A$. Thus, the average macroscopic field between the surfaces, $\overline{\delta E}$, equals $4\pi p/AL_x$. The resulting resistivity change, $\overline{\delta E}/J_0$, becomes

$$\delta\rho = \frac{4\pi p}{J_0 A L_x}, \tag{15}$$

which agrees with the result of Landauer's analysis [1, 2] for the resistivity per impurity for a slab consisting of a dilute concentration of random impurities. [The polarization field in that case equals $4\pi(N/AL_x)p$ for N impurities in a volume AL_x.]

Comparison of Equations (10) and (15) yields a relationship between force and resistivity, namely

$$\delta\rho = \frac{3\pi^2}{k_F^3 e}\frac{F_w}{J_0 A L_x}. \tag{16}$$

A relationship between the total resistivity change and the total force is expected on the grounds of momentum conservation arguments [9]. Here, however, we are considering only electron-wind contributions.

3. Impurity in a 2D electron gas

The analysis of the previous section can be extended to the case of a 2D electron gas. The current-carrying distribution is now a shifted Fermi circle, and has the form given in Equation (1). The asymptotic form of the wavefunction, in cylindrical coordinates, is

$$\psi_{\vec{k}}(\vec{\rho}) \rightarrow \frac{1}{\Omega^{1/2}}\left[e^{i\vec{k}\cdot\vec{\rho}} + \frac{f(\phi)e^{ik\rho}}{\rho^{1/2}}\right], \tag{17}$$

where the "volume" Ω is now the surface area of the 2D system. The calculation proceeds as before, where in Equation (4) dn/dE is now the 2D density of states $m/\pi\hbar^2$. The RRD potential becomes, in place of the expression (5),

$$\delta\Phi(\vec{\rho}) = -\frac{p\cos\phi}{\rho}, \tag{18}$$

where $\cos\phi = \hat{r}\cdot\hat{E}_0$ and

$$p = \frac{2\hbar}{k_F e} I_0 S_0. \tag{19}$$

Here I_0 is the 2D particle current density (current/length), and S_0 is the transport cross section:

$$S_0 = \int_0^{2\pi} |f(\phi)|^2(1 - \cos\phi)d\phi. \tag{20}$$

To determine the wind force on the impurity, we use the 2D forms of Equations (8) and (9). The calculation yields

$$F_w = ek_F^2 p, \tag{21}$$

which is the analog of Equation (10).

For the region where ρ is of the order of ℓ or greater, the solution of the transport equation (11) now yields

$$\delta n_w(\vec{\rho}) = \frac{me}{\pi\hbar^2}\frac{p\cos\phi}{\rho}, \tag{22}$$

which leads to the same $\delta\Phi$ as Equation (18) when the screening relation (4) is used.

An extra resistivity $\delta\rho$ is measured for an impurity between two parallel lines of length L_y separated by a distance L_x, where $L_y \gg L_x$. Averaging $\delta\Phi$ over the lines to find an average macroscopic field $\overline{\delta E}$, and using $\delta\rho = \overline{\delta E}/J_0$, where J_0 is the 2D electron charge current density, we obtain

$$\delta\rho = \frac{2\pi p}{J_0 L_y L_x}. \tag{23}$$

This is equivalent to the resistivity per impurity for a random, dilute concentration of N impurities in a 2D sheet of length L_y and width L_x, where $L_y \gg L_x$. (The polarization field equals $2\pi Np/L_y L_x$ for a sheet of 2D RRDs.)

4. An impurity near a surface

Consider an impurity inside a metal at a distance b from a flat surface, which we model by an infinite barrier potential. A current flows parallel to the surface. Far from the impurity, the current density $\vec{J}_0$ and the electric field $\vec{E}_0$ are uniform, with $\vec{E}_0 = \rho_0\vec{J}_0$ as in the analysis of Section 2. The presence of the surface introduces novel features in the RRD analysis.

When the impurity is farther from the surface than several electron wavelengths ($k_F b \gg 1$), the scattered waves emanating from the impurity are essentially the same as in the bulk case. This is also true for the momentum transfer, and consequently for F_w. The bulk limit obtains because scattered waves leaving the impurity and subsequently reflecting from the surface do not return to the impurity in sufficient intensity when $k_F b \gg 1$. Although F_w reduces to its bulk value, $\delta\Phi(\vec{r})$ does *not*. For example, consider an observation point, $\vec{r}$, well away from the impurity ($r \gg b$). The scattered waves directly from the impurity and the waves reflected from the surface after being scattered by the impurity arrive at $\vec{r}$ with essentially equal intensity. Therefore, the RRD strength is twice the bulk value (6) when $r \gg b \gg k_F^{-1}$.

When the impurity is very far from the surface ($b > \ell$), the problem is very simple. We need only consider a point RRD source at the impurity, and solve the transport equation subject to the boundary condition that at the surface there is no perpendicular component of current. Equivalently, the electric field $-\vec{\nabla}\delta\Phi$ at the surface must be parallel to the surface. The solution can be obtained by placing an image RRD outside the surface with both RRDs aligned parallel. Clearly, $\delta\Phi$ is again double strength in the far region where $r \gg 2b$.

When the impurity is very close to the surface ($k_F b \sim 1$), the quantum scattering interference between the impurity and the surface is essential. The scattered waves can be found by solving an equivalent image-scattering problem in which there is an incident wave $[\exp(i\vec{k}\cdot\vec{r}) - \exp(i\vec{k}^*\cdot\vec{r})]$, where $\vec{k}$ and $\vec{k}^*$ are image wavevectors. This wave is repeatedly scattered by the impurity potential and its image. After $\psi_{\vec{k}}(\vec{r})$ is found, the general method of Section 1 may be followed. $\delta\Phi$ exhibits non-dipolar angular dependence due to the directional dependence of the interference pattern when $\ell > r \gg k_F^{-1}$. However, for $r \gg \ell$, the leading term again has the dipolar form (5), except that p is replaced by some effective dipole moment which depends sensitively on b.

We performed model calculations for various quantities of interest in the case of a localized s-wave impurity potential near a surface. We found that for $r \gg \ell$ (but b arbitrary) the effective RRD moment is given by

$$p_{\text{eff}} = 2p\left[1 - \frac{3}{2}\frac{j_1(2k_F b)}{k_F b}\right]H, \tag{24}$$

where p is the bulk RRD moment (6), j_1 is the spherical Bessel function, and

$$H = \frac{1}{\sin\delta_0}\text{Im}\left[\frac{e^{i\delta_0}}{1 + ie^{i\delta_0}\sin\delta_0 h_0^{(1)}(2k_F b)}\right]. \tag{25}$$

Here δ_0 is the impurity phase shift and $h_0^{(1)}$ is the spherical Hankel function. Note that far from the surface $p_{\text{eff}} \rightarrow 2p$. Multiple scattering interference effects are contained in H.

The corresponding force is given by

$$F_w = \frac{2k_F^3 e}{3\pi}\, p_{\text{eff}}, \tag{26}$$

which is valid for all values of b. Note that the proportionality constant between F_w and the RRD strength p_{eff} is half the value which appears in the bulk expression (10).

The resistivity change for an impurity midway between parallel surfaces of area A separated by a distance L_x has the form

$$\delta\rho = \frac{2\pi p_{\text{eff}}}{J_0 A L_x}. \tag{27}$$

In obtaining Equation (27), we assumed that $A^{1/2} \gg L_x \gg b$, and that the surfaces are entirely within the metal. The importance of electrode geometry and boundary conditions has been emphasized by Landauer [10]. If noninvasive point probes rather than electrodes were used, one could, in principle, measure the RRD potential $-p_{\text{eff}}\cos\theta/r^2$ directly.

5. Conclusion

The RRD is the source of the long-range microscopic field associated with electron scattering by impurities in metals. The residual resistivity, $\delta\rho$, and the electromigration wind force, F_w, are directly related to the strength of the RRD, which thus provides a link between $\delta\rho$ and F_w. These relationships are generalizable to systems consisting of impurities near surfaces and interfaces. For the case of an impurity in a bulk 3D system or in a 2D system, the potential field is dipolar at distances beyond several electron wavelengths from an impurity. Because the field of a 2D dipole falls off more slowly with distance than that of a 3D dipole, the voltage drop across an impurity is larger in a 2D electron gas, assuming that the voltage probes are equally spaced in the two cases. For the case of an impurity in a metal at a distance b from a specular surface, the potential is dipolar at distances $r \gg \ell$. Closer in, however, the potential is not dipolar. The lack of an RRD field when $r < \ell$, even though $r \gg b$, is due to the antenna-like directional effect of the impurity plus image-scattering potential.

Finally, we point out that we have not considered local field contributions arising from the polarization of electrons brought in by the impurity in the presence of the electric field $\vec{E}_0$. Such effects enter the so-called "direct force" in electromigration theory [11] and have been described by Landauer [12] in terms of carrier density modulation. Formally, such effects are of order $1/k_F\ell$ times the electron-wind effects considered here, and can thus be neglected for good conductors.

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Richard S. Sorbello *University of Wisconsin–Milwaukee, Milwaukee, Wisconsin 53201.* Dr. Sorbello is Professor of physics and a member of the Laboratory for Surface Studies at the University of Wisconsin–Milwaukee. He received his Ph.D. from Stanford University in applied physics in 1970. Previously, he obtained B.S. and M.S. degrees from the Massachusetts Institute of Technology, Cambridge, in electrical engineering. From 1970 to 1973 he was a research associate at the Swiss Federal Institute (ETH) in Zurich. Dr. Sorbello's research interests include electronic transport theory, electromigration, and dynamical processes at surfaces and interfaces.

C. S. Chu *University of Wisconsin–Milwaukee, Milwaukee, Wisconsin 53201.* Dr. Chu received his B.A. in physics from the Chinese University of Hong Kong. He then enrolled in the physics department of the State University of New York at Buffalo, joined the research group of Professor Y. C. Lee, and performed theoretical studies in the electronic responses in low-dimension systems. Dr. Chu received his Ph.D. from SUNY at Buffalo in February 1987. Since then, he has been working on the electromigration and transport problem in microstructures in the group of Professor R. Sorbello at the Laboratory for Surface Studies at the University of Wisconsin–Milwaukee.