Driving force in electromigration

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The driving force in electromigration is generally assumed to consist of a "direct force" due to the applied field and an "electron-wind" term due to momentum exchange with the current carriers. In the case of the "direct force" it is uncertain how effectively the charge is screened. In the case of the "electron wind" it is unclear whether the moving atom senses the carrier's change in lattice momentum or real momentum. A method first utilized by Bosvieux and Friedel, and expanded by Sorbello, resolves these problems by calculating driving forces on the unscreened ion resulting from the nonuniformities in spatial carrier distribution. These theories depend, however, on an incomplete picture of the spatial variations in the electric field, which inevitably accompany current flow past localized scatterers. Furthermore, "screening" of the charge of a lattice defect is related to inhomogeneities in carrier density and the resulting spatial inhomogeneity in the rate of current production which a uniform field would provide. Terms of this latter sort have never received explicit consideration.

I. INTRODUCTION

The transport of matter through metals in the presence of a dc current, known as electromigration,[1] has a long history, and has recently become technologically important as a potential source of component failure in integrated circuits.[2] The conceptual understanding of the process started in 1907 with Skaupy, who recognized that the moving conduction electrons can drag atoms along through a frictional force. A series of modern publications[3-7] has contributed considerably to this clarification, and has culminated in a significant recent paper by Sorbello.[8] Despite these advances, we believe that there are some very basic points which are still unappreciated, and we will try to make these points in this article at the simplest possible conceptual level.

Electromigration in bulk crystals is found to occur for solute atoms as well as for the host metal. In the latter case it is, of course, a vacancy that is driven in a direction opposite to that of the observed motion of matter. To cover both vacancy and impurity motion with one phrase, we shall refer to "lattice inhomogeneities." It is easiest, however, to think about the case of an interstitial ion, and our language will reflect an implicit emphasis on that case.

An observed rate of atomic drift can generally be regarded as a consequence of two factors: a mobility and a driving force. We shall, in this discussion, be concerned exclusively with understanding the driving force. There are, of course, serious problems also involved in understanding the mobility, e.g., the effects of correlated motion for several types of lattice defects.[9]

In studies of the force term, it has been customary to distinguish two types of contribution: that from the scattering of the electrons by the ion in question (the electron-wind term) and that from the direct interaction of a local charge with the applied field (the direct force).

Consider first the electron-wind force. Fiks[3] and Huntington and Grone[4] have calculated this force by considering the momentum exchange between the impurity ion and the electronic current. In this approach, it is necessary to decide how the momentum exchanged in a scattering event is shared between the impurity ion and the lattice. This is equivalent to the question: Does the scatterer "sense" the carrier's change in lattice momentum or the change in real momentum or some compromise of the two? This is a difficult question and it is not clear that it has been adequately resolved.

Similar physical uncertainties turn up in the direct-force term. The impurity is in a dense electronic medium, and is tightly screened. If there were no current flow present, then the screening charge would have to move with its impurity, and the moving entity would be clearly neutral. It is in fact possible to have electric fields, without simultaneous currents, produced for example by strain gradients. In that case[10] it is believed that the electric fields do not provide a driving force for atomic motion. Huntington[6] has, however, particularly emphasized that in the presence of electronic current flow it is not clear that the screening cloud really moves along with the impurity.

An alternative approach to these physical difficulties was initiated by Bosvieux and Friedel,[5] continued by Gerl,[7] and most recently extended by Sorbello.[8] Their basic point is that we should calculate the forces on the unscreened bare ion. This bare ion is characterized by essentially the same mobility as the screened ion. The forces on the bare ion can be calculated by taking into ac-

count all the charge disturbances accompanying the electronic transport process, and then finding the interaction between these disturbances and the bare unscreened ion. These charge disturbances include those caused by the ion under consideration, those centered about other ions, and those at the ends of the specimen and responsible for the uniform field. Under this viewpoint, we can *explicitly* assert that screening, *if it exists*, must be manifested in the local conduction-band charge nonuniformities near the obstacle.

Sorbello[8] invokes pseudopotential techniques. His calculation is thus not nearly as dependent on an assumption of weak electron-ion scattering as the earlier work of Bosvieux and Friedel[5] (hereafter called BF) and of Gerl.[7] Our discussion will be oriented toward impurities in a uniform electron gas (rather than the complexities of pseudopotentials), and therefore relates more directly to the "jellium" calculations of BF. The basic ideas, however, *also* apply to the work of Sorbello.

The BF theory and its subsequent elaborations attempt to calculate the charges piled up in the vicinity of an impurity. This is a part of the overall force calculation. To make our own subsequent points clear, it will be useful here first to discuss those terms of the BF theory which agree conceptually with the terms also invoked by Sorbello.[8] These are terms which result from following the motion of the incident carriers, in the presence of a current distribution, past the scattering center. As a result of the deflection by the scattering center, carriers are deflected preferentially into some parts of space and charge inhomogeneities result.

II. POLARIZATION DUE TO THE SHIFTED FERMI SPHERE

A single point charge Ze is placed at the origin in an otherwise uniform electron gas of density n, and in an externally applied field $\vec{E}_{ex}$. Additional uniform background scattering is assumed to exist, depending only on the angle through which the carrier is scattered, and thus gives rise to a characteristic time τ for current decay. BF's localized conduction-band charge disturbance $\delta\rho(\vec{r})$ consists of three terms, $\delta\rho_0 + \delta\rho_1 + \delta\rho_2$, each to be discussed separately. $\delta\rho_0$ is the static screening of the ion in question in the absence of current flow and exerts no force on the ionic point charge. The ion in question and the screening charge $\delta\rho_0$ together determine a self-consistent field which scatters incident carriers. Far from this ion the current is uniform, and the distribution in $\vec{k}$ space, $f(\vec{k})$, is the usual shifted Fermi sphere. This shifted Fermi distribution in the absence of a localized scatterer prevails uniformly throughout the space of the sample and corresponds to the same charge density as the original unshifted equilibrium distribution.

Near the impurity the current carriers are scattered and the charge changes due to the motion of the scattered carriers are given by $\delta\rho_1$. These piled-up charges in turn are screened by an additional charge distribution $\delta\rho_2$ which is not associated with any current flow. BF calculated $\delta\rho$ to first order in the self-consistent potential V which exists in the presence of current flow. The Born approximation is used to determine $\psi_{\vec{k}}$, the wave function for a scattered carrier with incident momentum $\vec{k}$. $\delta\rho$ is then given by weighting these changes with the incident distribution $f(\vec{k})$,

$$\delta\rho(\vec{r}) = \sum_{\vec{k}} f(\vec{k})\,(|\psi_{\vec{k}}|^2 - |\phi_{\vec{k}}|^2)\,. \tag{1}$$

$\phi_{\vec{k}}$ is the eigenfunction at zero V and $\vec{E}_{ex}$. The above expression is then calculated to *first order in* V, and thus emphasizes the interference terms between incident wave and scattered wave. Equation (1) as written differs, in fact, from the strict prescription given in BF by terms which are second order in the applied field. (The reader should note that we have just referred to the externally applied field, not to the scattering potential.) We are concerned, however, only with effects proportional to $\vec{E}_{ex}$. BF found that the asymptotic expression for $\delta\rho_1$ is

$$\delta\rho_1(\vec{r}) \sim -\lambda\,(k_F/2\pi^2)\,\tau\,\vec{E}_{ex}(\vec{r}/r^3)\sin(2k_F r), \quad \text{as } r\to\infty. \tag{2}$$

λ is a constant indicating the strength of the scattering potential; it is proportional to the charge Z. $\hbar k_F$ is the Fermi momentum.

The force on the point ion due to $\delta\rho_1 + \delta\rho_2$ associated with it is then found to be

$$\vec{F}_e^{\,1} = -e\vec{E}_{ex}\,\Delta\rho/\rho_0, \quad \Delta\rho = S_0\,\hbar k_F/e^2\,, \tag{3}$$

where S_0 is the transport scattering cross section of the impurity, and ρ_0 is the unmodified host resistivity. In our notation the additional resistivity produced by a density of N ions is $N\Delta\rho/n$. BF show that this result agrees with the momentum-exchange term predicted by the Fiks-Huntington approach. Indeed, for the simple model under consideration, an impurity ion in jellium, the momentum-vs-pseudomomentum question does not arise since there is no lattice.

III. RESIDUAL RESISTIVITY DIPOLES

Section II summarized the BF calculation of the electron-wind force. BF utilized the Born approximation and calculated $\delta\rho$ to first order in the scattering potential V. Their $\delta\rho$ is an oscillating function of r. In this section, we consider contributions which are of order V^2. These contribu-

tions do not exhibit the rapid oscillations of $\delta\rho_1$ in Eq. (2). The result is that the contribution of these V^2 terms to the field at the ion site may be of the same order of magnitude as the first-order terms considered in Sec. II.

A calculation very similar in spirit to that of BF in calculating $\delta\rho_1$ was first carried out by one of the authors of this article[11] some years before the appearance of BF. This earlier calculation was semiclassical and did not permit interference terms of the type which are the basis of BF's $\delta\rho_1$. The earlier calculation dealt with the details of the spatial variation for transport in the presence of localized scatterers. Consider a block of homogeneous copper, 1 m along each edge, carrying a uniform current density. Now introduce one localized scatterer into this block, keeping the total current flow through the block constant. Since the resistivity has gone up, the voltage across the block must have increased. It seems most unlikely that the increase in field, i.e., the residual resistivity field, is uniform. The spatial distribution of the residual resistivity field *must* be related to the location of the scattering center. The simplest localized field with a nonvanishing average is a dipole field. These residual resistivity dipoles were studied in detail in Ref. 11 and found to account for the total increase in average field required by more conventional theories. While the actual calculation in Ref. 11 is somewhat complex, the main result is not. Roughly speaking, one can think of the incident carriers piling up against the scattering center and building up a dipole until the dipole potential becomes big enough to move the carriers around the scattering center, almost as if the localized scatterer were a macroscopic inclusion of poorly conducting material. The charge density responsible for the dipole field will be called $\delta\rho_p$.

This theory of residual resistivity dipoles[11] not only is approximate in its semiclassical nature, but also in its replacement of the actual scattering center by a point scatterer with the correct differential cross section. It thus does not do justice to the exact path taken by the scattered carriers in the immediate vicinity of the scattering center. The exact path is, presumably, handled more correctly in the BF theory. Since, however, the residual resistivity dipoles account correctly for the total required increase in field, the details of the motion in the immediate vicinity of the scattering center can only generate higher-order corrections to the residual resistivity dipoles, i.e., more rapidly oscillating fields. In the residual resistivity dipole calculations, as in Sec. II, $\delta\rho_p$ consists of two terms, $\delta\rho_{p1}$ and $\delta\rho_{p2}$. $\delta\rho_{p2}$ is the screening for $\delta\rho_{p1}$, which in turn is determined by the carriers present in nonequilibrium numbers and deflected out of the incident distribution into new directions. Thus we find $\delta\rho_p$ proportional to differential scattering cross sections and therefore *proportional to second and higher powers of the scattering potential.* In contrast to Eq. (2) $\delta\rho_p$ does not change sign with Z. In fact, as already pointed out, the field associated with the residual resistivity dipoles is the residual resistivity field; i.e., on the average it is always in the direction of current flow.

To find the residual resistivity dipole $\vec{p}$, consider a density N of identical scatterers per unit volume. Let N be small enough so that the scatterers are essentially noninteracting and the overall resistivity remains dominated by the uniform thermal scattering. The polarization per unit volume will then be $N\vec{p}$ and the space average of the associated field is $\vec{E}_{\text{dipole}} = -4\pi N\vec{p}$. This is just the additional field needed to drive the current $\vec{j}$ past the obstacles, i.e., $\vec{j}\, N\Delta\rho/n$. Hence, we find

$$\vec{p} = (\Delta\rho/\rho_0)\,(\vec{E}_{ex}/4\pi n)\,, \tag{4}$$

where $\Delta\rho$ and ρ_0 are defined as in Sec. II and n is the conduction electron density.

To evaluate the contribution of the residual resistivity dipoles to $\vec{E}_{loc}$, the field at the ion site, we must know more than the magnitude of the dipole moment; we must also know where the charges which constitute the source of that dipole moment lie. If we were really dealing with a point scatterer, then the dipole source charges would lie within a screening length l_s of the scattering center. If the scattering potential is distributed over an atomic volume, then we would expect the charges to be distributed over a sphere which goes bevond the atomic volume by a screening length. Actually, in fact, the *self-consisent* potential of the scatterer, in the absence of transport, already extends beyond the volume of the scatterer because the screening electrons are more widely distributed than the original differences in atomic potential. As a crude guess, let us take the dipole source charges as concentrated on a surface l_s away from the impurity-ion core surface. If they are less concentrated in space for the same net dipole moment, then the field will be smaller. The core radius is of the order of a Bohr radius a_0, and l_s depends on the density of states at the Fermi surface.

Now a dipole of moment $\vec{p}$ deposited on a sphere of radius a will give a field inside the sphere

$$\vec{E} = -\vec{p}/a^3. \tag{5}$$

Combined with Eq. (4) this yields a field at the ion site

$$\vec{E}_{loc}^{(p)} = (\Delta\rho/\rho_0)(1/4\pi na^3)\vec{E}_{ex}$$
$$= \tfrac{1}{3}(\Delta\rho/\rho_0)\vec{E}_{ex}(r_s a_0/a)^3 , \quad (6)$$

where $\frac{4}{3}\pi(r_s a_0)^3$ is the volume per electron. For a system at room temperature, l_s can be evaluated in the Fermi-Thomas approximation. For $r_s = 3$ and mass of the electron equal to the free-electron mass, $l_s \simeq a_0$ and hence $a \simeq 2a_0$. Thus, we find

$$\vec{E}_{loc}^{(p)} \simeq (\Delta\rho/\rho_0)\vec{E}_{ex}$$

and (7)

$$\vec{F}_e^{(p)} \simeq Ze(\Delta\rho/\rho_0)\vec{E}_{ex} .$$

We see that this is comparable to the BF term of Eq. (3). For a more realistic model, the scatterer may well be more extended in space, particularly if we take into account the elastic distortions produced by the lattice inhomogeneity. The greater spatial extent will reduce $\vec{F}_e^{(p)}$.

We have shown that the second-order contribution given by Eq. (7) can be comparable to the first-order one given by Eq. (3). This leaves the size of still-higher-order terms uncertain. When we examine the ratio of charge densities rather than forces, the first-order terms of BF are in fact (as one might expect) large compared to our $\delta\rho_p$. It is only after integrating over volume to calculate a force that the second-order terms become comparable, because the second-order charge density is not an oscillatory one. This feature, however, can be invoked only once; the third-order terms in V cannot be "less oscillatory" than the second-order terms.

IV. ADDITIONAL SOURCES OF LOCAL FIELDS: SCREENING

Sorbello[8] asserts that the local fields discussed in Sec. II are the only local fields. In his treatment, in addition to the forces caused by the charge accumulations of Sec. II, the bare ion is exposed to the uniform background field, whose sources can be taken to be at the boundaries of the specimen. Thus, if the Sec. II forces can be labeled electron-wind forces, then Sorbello has the bare ion exposed additionally to the unscreened background field.

Sorbello essentially agrees in this with Huntington,[6] who argues that the motion of the screening electrons, which compensate for the bare ionic charge, is the important factor. Huntington thus emphasizes the motion of the essentially symmetrical screening charge whereas BF emphasize the asymmetry of the local charge and the resulting force on the bare ion. Huntington argues that the "screening electrons" do not follow the impurity motion. Hence, they are ineffective in screening out $\vec{E}_{ex}$, the uniform background field. Huntington's arguments depend upon a particular "gedanken" experiment,[6] in which the electrons do not follow the impurity. Huntington's argument undoubtedly does show that screening electrons do not absolutely have to follow the ion with which they are associated. It is unfortunately not equally clear that his "gedanken" experiment, which involves ions being taken in and out of the specimen and in fact far away from the specimen, is closely related to the particular sequence of events in the real electromigration situation. BF, on the other hand, claim that for an interstitial impurity, screening is completely effective in eliminating the "direct force," while for a substitutional impurity the deviation in charge from the host lattice is supposedly screened and ineffective. In other words, the deviations in charge from the unperturbed lattice are screened. That is essentially a generalization of the conclusion of Ref. 10, which confines its attention to substitutional impurities. Reference 10, however, only applies to the case of a field unaccompanied by current, and not to an open system.

BF's calculation of screening charge proceeds by applying perturbation theory to the ground state, in the presence of a field but without a current. It is not clear (to the present authors at least) that such a treatment has any bearing on the distribution of charge in a dissipative current-carrying open system. The accumulation of charges in the presence of current flow must be such as to give rise to a field which in turn causes a current pattern providing continuity of current. This is analogous to the calculation of voltage distribution in a network of resistors in which each resistor is paralleled by a capacitance. In the steady state it is only the resistors (i.e., the transport effects) which determine the potential distribution. Thus we fail to see how the BF screening fields, calculated from ground-state polarization effects without regard to scattering effects (resistors), can be relevant. Despite this criticism we shall see that there are arguments for an additional screening charge which has some resemblance to the BF results.

Let us first consider, as a sample problem, an isolated hydrogen atom in space. In the presence of a field it becomes polarized. As a result the nucleus "sees" the applied field as well as the field due to the polarization of the electron, and these cancel, resulting in complete screening. The screening is complete just as if the nucleus were imbedded in a conducting sphere which in turn is inserted into a region with a uniform field. The field disappears from the region in which there are readily displaceable charges and becomes concentrated in the region devoid of such charges. It is immediately apparent that our case is different.

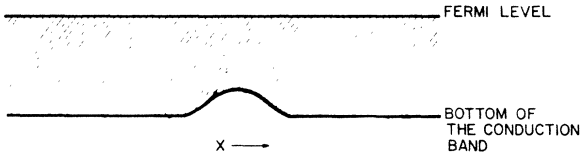

FIG. 1. One-dimensional model of a repulsive lattice inhomogeneity, creating a region of lowered carrier density.

All of the metal is conducting; we are not dealing with an impurity atom in empty space. It is true that the immediate vicinity of the impurity atom has a greater or lesser density of carriers in it, and therefore we can expect the applied field to be modified. The field will be reduced if the carrier density is larger in the vicinity of the impurity but increased in the case of a repulsive impurity.

Let us go through a highly oversimplified calculation to suggest that such terms really do exist. Consider a one-dimensional system as shown in Fig. 1, with a localized bump representing a repulsive lattice inhomogeneity. The extra scattering due to the bump has already been considered in earlier sections; here we are concerned with the effects of the variable carrier density, and will assume that there is a spatially uniform background of lattice scattering. (A clear separation of carrier-density inhomogeneities from scattering effects is possible only in our semiclassical one-dimensional model.)

Consider first current flow in the absence of any lattice scattering. Let n_+ and n_- be the respective densities per cm of right-moving and left-moving electrons within some modest energy range at the Fermi surface. Then the current $j = -ev_F(n_+ - n_-)$, where v_F, the magnitude of the velocity at the Fermi surface, is a function of x. Continuity of current will exist, and therefore $n_+ - n_- \propto 1/v_F(x)$. Now turn on a spatially uniform but incoherent lattice scattering (Einstein scattering) characterized by a relaxation time τ. This will cause the carrier imbalance $n_+ - n_-$ to start decaying as $e^{-t/\tau}$. Now, however, if we apply a field $E(x)$, it will generate a carrier imbalance locally at a rate proportional to $(\partial n/\partial k)(dk/dt)$. In one dimension $\partial n/\partial k$, the density of states at the Fermi surface, is independent of x. The electron acceleration term dk/dt is proportional to $E(x)$. Thus, if $E(x) \propto 1/v_F(x)$, the carrier imbalance initially present can be maintained. Hence very localized field nonuniformities can come into existence and must be added to those discussed in earlier sections. We do not put this forth as a serious analysis of screening, but only as an argument to point out that the terms related to a *spatially nonuniform rate of current generation* by a uniform field do exist. Note, however, that our discussion does do justice to the nonvanishing size of the mean free path; it is not a macroscopic treatment averaging over regions comparable to a mean free path. We have used a Fermi-Thomas type inhomogeneous electron-gas picture. This is much more likely to do justice to the case in which no bound charges are involved in the screening process than in the case where an attractive impurity potential is deep enough to trap a conduction electron.

Despite their apparently very different origin, the fields we have just discussed do resemble the BF screening fields resulting from an equilibrium calculation. Consider a region in which a smeared-out ionic charge density $\rho_I(x)$ varies slowly, and differs from its value in the unperturbed metal. If the scale of variation of $\rho_I(x)$ is slow compared to the screening length in the metal, then the compensating equilibrium electronic-charge density $n_0(x)$ will be proportional to $\rho_I(x)$. In the simplest possible case of constant effective mass, the Fermi velocity $v_F(x)$ will then also be proportional to $\rho_I(x)$. $E(x)$ will then, in turn, be inversely proportional to $\rho_I(x)$. The force per unit length $\rho_I(x)E(x)$ on the bare ionic material will be independent of ρ_I, and will equal the value in the undisturbed surrounding matrix. Thus the deviation from the undisturbed matrix will be screened, as in the BF theory. We have had to make a great many approximations to get this result, but it is not clear that all of these are necessary. Thus, in this discussion, we have emphasized a very slowly varying ionic and electronic charge distribution. At the other extreme, however, where a deviation in ionic charge is neutralized by bound states drawn well out of the conduction band, one would again expect the deviation in ionic charge to be screened against the effect of an applied field.

In conclusion we wish to point out that we have only discussed the effect of an electric-field inhomogeneity on the particular lattice inhomogeneity responsible for that field. As Sorbello makes very clear, there are interactions; one inhomogeneity "sees" the fields produced by others. As far as the long-range dipole terms are concerned this leads to situations related to the Lorentz correction. The role of Lorentz corrections in the residual resistivity problem has already been emphasized in an earlier paper.[12]

Note added in proof. Das and Peierls[13] have recently supplied an additional analysis of the electromigration problem. They calculate electronic charge disturbances to first order in the perturbation potential and, as a consequence, the residual resistivity dipoles are not included. The Das-Peierls analysis is more consistently classical than the original discussion of residual resistivity dipoles.[11] In contrast to that analysis Das and Peierls do not assume a differential scat-

tering cross section, but invoke classical laws of motion, through the Boltzmann equation, to calculate particle deflections. Within these assumptions we believe that their analysis is correct and consistent, and does not require *ad hoc* superposition of terms as in BF.[5] We believe that the Das-Peierls calculation includes the conductivity modulation effects discussed in our Sec. IV above, despite verbal insistence by Das and Peierls that their calculation demonstrates the absence of screening effects.

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