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ZEE STAR ANALYSIS

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Forces contributing to the effective valence Z* in electromigration have been theoretically studied for the following systems: An impurity in the vicinity of a grain boundary, an impurity in the vicinity of a dislocation, and impurity in a disordered system. The presence of a grain boundary or dislocation was found to change Z* and the residual resistivity by an amount on the order of 10% to 50%. The local transport field in mesoscopic systems was investigated, and the calculations suggest that the scanning tunneling microscope can effectively probe this field. Non-adiabatic recoil effects in the wind force exerted on an impurity were also considered.

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I. INTRODUCTION

The main objective of our research program was to obtain a better theoretical description of the forces contributing to the effective valence Z^* in electromigration. Quantum mechanical and classical analyses were made in order to develop an improved understanding of Z^* for impurity ions in mesoscopic and sub-mesoscopic structures. This study was undertaken to develop insights that will lead to a better understanding of the electromigration failure mechanism in metallic interconnects.

The major contribution to the electromigration driving force arises from the "electron wind" impinging upon the impurity-ion and transferring momentum to it. This is the so-called electron-wind force.[1] A proper evaluation of the electron-wind force for a general defect configuration requires a calculation of the local transport field[2] in the region of the mobile impurity ion. This local field is caused by the self-consistent screening of the electron pile-up as the incident electrons are scattered by the defect.[2]

We have investigated the electron wind force and the local transport field for the configurations of an impurity in the vicinity of a grain boundary and in the vicinity of a dislocation. We set up the theoretical expressions for the case that the current is perpendicular to the grain boundary and for the case that the current is perpendicular to the dislocation axis. This study complements our previous investigation for the same systems, where we had taken the current to be parallel to the grain boundary and to the dislocation axis.[3] The perpendicular orientation is the more difficult one to analyze, and the calculations reported here are the first ones reported for this problem.

Another system which was considered was that of a localized weak-scattering impurity in an electron gas that is characterized by incoherent background scattering and a relaxation time τ in the density-matrix formalism. The usefulness of the density-matrix approach is that it allows a more realistic model of background scattering, taking into account the smearing of electronic energy levels and the microscopic changes in the chemical potential. This has relevance in trying to establish a self-consistent picture of electron transport in the presence of both elastic scattering by impurities and inelastic scattering by background phonons.

An important question concerns the possibility of measuring the local transport field by a weakly-coupled probe such as the scanning tunneling microscope (STM). The STM probe effectively represents a weakly-coupled metallic lead attached to the mesoscopic system. By varying the STM voltage

so as to keep the tunneling current in the STM tip constant as the tip is moved across the surface of the mesoscopic system such as an ultra-thin film, one can effectively probe the local transport field. At least this is the claim made by Kirtley et al.[4] We previously investigated this claim using an approximate analysis[5] in which the phase-sensitivity of the STM measurement was neglected. We have re-examined this issue using a more elaborate theory, and we have been attempting to extend the theoretical analysis to the system of an impurity in the vicinity of a metallic surface.

The problem of the recoil of an impurity exposed to bombardment by an electron beam was also considered. We considered classical and quantum mechanical analyses following the approach outlined in our earlier report[3] and tying together some important loose ends in our theory. Of specific concern was the role of non-adiabaticity in modifying the wind force in the classical and quantum mechanical regimes.

II. IMPURITY NEAR A GRAIN BOUNDARY

Consider an impurity at a distance z from a grain-boundary in the jellium model. The grain boundary is modelled as a repulsive barrier of height U and thickness d, centered at z = 0. This grain boundary model was used previously by others[6] and more recently by us in treating the problem of an impurity outside a grain boundary for the case that the electron current is parallel to the grain-boundary.[3] The model ignores the details of the lattice mismatch at the boundary, but instead replaces the grain-boundary region as a repulsive barrier because of the loose mis-fit of atoms in that region.

The wind-force exerted on the impurity at position $\vec{R}$ can be written as

$$\vec{F}_w = -\int \delta n_w(\vec{r}) \frac{\partial V}{\partial \vec{R}} d^3r \ , \tag{1}$$

where $\delta n_w(\vec{r})$ is the electron density pile-up due to the electron wind and V is the impurity potential. For a given incident electron distribution $g_{\vec{k}}$, we have[2]

$$\delta n_w(\vec{r}) = \sum_{\vec{k}} g_{\vec{k}} \, |\psi_{\vec{k}}^{(+)}(\vec{r})|^2 \tag{2}$$

where $\psi_{\vec{k}}^{(+)}(\vec{r})$ is the scattering-state wavefunction which evolves from the incident plane-wave state $\exp(i\vec{k}\cdot\vec{r})$. The impurity potential is modeled as an attractive short-range potential, which we write in the delta-function form $V(\vec{r}) = -v_o \delta(\vec{r}-\vec{R})$, where v_o is a positive constant.

The total residual resistivity of the complex can be written in the form

$$\delta\rho = \rho_{imp} + \rho_{GB} + \Delta\rho(\vec{R}) \ , \tag{3}$$

where ρ_{imp} is the resistivity due to an impurity in bulk, ρ_{GB} is the grain-boundary resistivity, and $\Delta\rho(\vec{R})$ is the additional resistivity due to interference effects between the grain boundary and the impurity. It is interesting to note that for the parallel configuration $\rho_{GB} = 0$ within our model, and that $\Delta\rho(\vec{R})$ is of order v_o^2 in the impurity potential. For the perpendicular case $\rho_{GB} \neq 0$ and $\Delta\rho(\vec{R})$ is of order v_o.

We have obtained analytic expressions for the resistivity and for the wind force assuming the Born approximation limit of weak potentials. Preliminary numerical calculations reveal that when the impurity is within a few angstroms of the grain boundary, the interference term is appreciable and a de-enhancement of the resistivity and wind-force on the order of 50% occurs when the impurity enters the grain boundary region ($|z| < d/2$). From this result it follows that an impurity which hops into and out of a grain boundary can give rise to resistivity fluctuations on the order of $\frac{1}{2}\rho_{imp}$. This size resistivity fluctuation is of the correct magnitude to explain recent 1/f-noise data.[7] It is interesting that the resistivity fluctuation occurring here for the perpendicular orientation is of the same order as for the parallel orientation treated previously.[3] There is also a corresponding reduction in the electron wind force on the impurity when it is in the grain boundary. However, unlike the case for the parallel configuration, the reduction in wind force is not due to the impurity being shielded against the electron wind by the grain boundary. Rather, the mechanism in the perpendicular configuration is that the induced near-field dipole field surrounding the grain boundary exerts a corresponding back-force on the impurity. There is no shelter from the electron wind because the wind "blows" through the grain boundary in the perpendicular configuration, this being a consequence of current conservation.

III. IMPURITY NEAR A DISLOCATION

We have also considered the problem of an impurity at a position $\vec{R}$ relative to the axis of a dislocation within the jellium model. The electron current is taken to be perpendicular to the dislocation axis, and the dislocation is modeled as a barrier of height U and radius a. The calculation complements our previous treatment[3] in which the current was

taken to be parallel to the dislocation axis. The impurity potential is again modeled as an attractive delta function $V(\vec{r}) = -v_o \delta(\vec{r}-\vec{R})$.

For the total residual resistivity of the impurity plus dislocation complex, we have in place of Eq. (3), the expression

$$\delta\rho = \rho_{imp} + \rho_{disloc} + \Delta\rho(\vec{R}) \ , \tag{4}$$

where ρ_{disloc} refers to the residual resistivity contribution of the isolated dislocation (in the absence of the impurity).

The dislocation problem is similar in many respects to the grain boundary problem of Sec. II. In particular, $\rho_{disloc} = 0$ for the case that current flow is parallel to the dislocation and is non-zero for the perpendicular orientation. Furthermore the interference term $\Delta\rho(\vec{R})$ is found to be appreciable only within a few angstroms of the dislocation, and is of order v_o for the configuration of perpendicular current flow.

Numerical calculations indicate that $\Delta\rho(\vec{R})$ can fluctuate by an amount on the order of $\frac{1}{2}\rho_{imp}$ as the impurity jumps into and out of the dislocation core ($R < a$). This is also in qualitative agreement with the size of resistivity fluctuation required to explain recent 1/f-noise data in thin films.[7]

IV. DENSITY MATRIX CALCULATION

Recent experiments[8] on the electromigration of hydrogen in heavily disordered alloys indicate that the electromigration direct force is unity, whereas in the weakly disordered alloys the direct force departs from unity by about ±50% depending on the alloy. This has spawned a theoretical paper by Lodder,[9] who claims that in the absence of appreciable disorder there is complete screening of the direct force, whereas for large disorder one recovers the bare valence Z. (For hydrogen Z = 1.) Lodder claims to explain the hydrogen experiments, and in the process casts doubt on previous treatments of electromigration, especially on the work of Landauer. The response by Landauer[10] was swift and amounts to a vigorous dismissal of Lodder's work. Nonetheless the problem remains, what is the role of disorder in electromigration?

To obtain an answer to this question we employed a density matrix analysis in which the disorder is simulated by a background relaxation time τ on the right hand side of the Louiville equation. We evaluated the density matrix in the weak-scattering limit, following the number-conserving

relaxation-time approximation of Mermin and originally used in the electromigration problem by Schaich.[11]

The result for Z^* can be written in the form

$$Z^* = Z - Z^2 f(\tau) \tag{5}$$

where the function $f(\tau)$ is a complicated integral depending only on τ and the Fermi energy ϵ_F. The second term on the right-hand side of Eq. (5) is proportional to the square of the bare valence, i.e., it is formally linear in the strength of the scattering cross-section. It is then tempting to conclude that this term is the electron-wind force contribution and that therefore the first term, Z, is the remaining direct force. However for large τ, we find that $f(\tau) = C\epsilon_F\tau[1 + (\epsilon_F\tau)^{-1}]$, where C is a constant. In this case, we evidently have

$$Z^* = (Z-CZ^2) - Z^2 C\epsilon_F\tau \tag{6}$$

with the alternative interpretation that the wind force contribution is $-Z^2C\epsilon_F\tau$ and the direct-force valence is $Z-CZ^2$ rather than Z. The term $-CZ^2$ can be thus regarded as a second-order (in Z) screening correction to the bare valence contribution to the direct force.

We also find that for small $\epsilon_F\tau$, which would be appropriate to the strong disorder limit, $f(\tau)$ has the form $f(\tau) = D[1 + \epsilon_F\tau]$, where D is a constant. Therefore in this limit

$$Z^* = (Z-DZ^2) - Z^2 D\epsilon_F\tau \ . \tag{7}$$

In this case we see that the apparent direct force $(Z-DZ^2)$ for strong disorder will differ from the apparent direct force $(Z-CZ^2)$ for weak disorder. This may afford a clue to the variation in the experimentally deduced direct force in the hydrogen experiments. Preliminary calculations for the jellium model give values of C and D which are each of order 0.05 and hence would not account for the large experimental difference that were observed.

V. SCANNING TUNNELING MICROSCOPE AND THE LOCAL TRANSPORT FIELD IN MESOSCOPIC SYSTEMS

The local transport field is the self-consistent microscopic electric field that is set up in a current carrying conductor. It is this same field which exerts a force on the nucleus of an impurity ion and thereby gives rise to an electromigration driving force. We have investigated the possibility of whether this local transport field can be directly probed by a scanning

tunneling microscope placed just outside a mesoscopic system. If this were possible, the STM could be a useful, independent probe of electromigration forces. We have previously addressed this problem in an approximate analysis[5] which ignored the phase-sensitivity of the STM measurement. Recently, it was claimed by Büttiker[12] that phase-sensitivity is a very important feature of the STM measurement and that in the case of 1-d systems, at least, it is a dominant effect.

Since a calculation of STM potentiometry should in general include the phase-sensitivity of the probe we generalized our previous calculation[5] to include these effects. We considered the case of a grain boundary in a thin film and the case of an impurity in the vicinity of a surface.

We found that the phase-sensitivity of the STM voltage measurement gives rise to spatial variation of the STM voltage as the STM tip is moved away from a scatterer in a current-carrying system. The STM tip turns out to be a weak-coupling probe which does not couple equally to all propagating channels, but is more sensitive to higher subbands, i.e., to those modes of the mesoscopic system which have higher momentum component (i.e., more rapid spatial oscillations) toward the surface on which the STM tip resides. However, we found from explicit numerical calculations that the STM can still be used as a qualitative probe of the spatial profile of the local transport field. The phase-sensitivity of the STM measurement is not so pronounced as found by Büttiker for 1-d systems.[12] Preliminary estimates indicate that a 200 μV STM voltage drop is possible across a grain boundary subjected to a transport current density on the order of 10^7 A/cm^2 in an ultra-thin film. This is in accord with experimental values.[4] However, spatial oscillations having amplitudes on the order of 20 μV as in the experiments of Kirtley et al.[4] are not consistent with STM voltage patterns predicted by our theory. It is likely that some spurious effects are being observed in these experiments. Further experimental and theoretical work is called for, especially for systems containing impurities in the vicinity of a surface.

VI. RECOIL ENHANCED ATOMIC MIGRATION

Follow-up studies were made on our previous theory of recoil-enhanced atomic migration.[3] We found that the driving force for atomic migration, and specifically for electromigration, can be significantly affected by atomic recoil. Our classical theory is based on the approach-frequency picture as opposed to the thermodynamic equilibrium picture. We have investigated this question and believe that the approach-frequency picture is the better

picture in that the presence of the incident electron beam vitiates the purely thermodynamic considerations.

There are additional subtleties in going beyond the adiabatic approximation, as found for example, By Kondo[13] for the quantum-tunneling portion of an atomic jump. These corrections were described by Kondo in terms of renormalization effects, and they arise because the many-body electron ground-state when an impurity is at site A is orthogonal to the corresponding state when the impurity is at site B. As pointed out by Kondo,[13] this is related to "Anderson's orthogonality catastrophe." Upon study of this question we have concluded that these effects are associated with the equilibrium electron gas, whereas our treatment concerns the non-equilibrium part of the electron gas, i.e., the bombarding electron flux. As a first approximation, when the equilibrium effects are significant they can be included by re-normalizing the physical parameters of the system in the absence of the electron flux, and these renormalized quantities would be the relevant inputs for our analysis. For example, these inputs include the effective mass and oscillation frequency of an impurity in its potential well. These points were included in the final revised manuscript on this work which was submitted to Physical Review Letters, and which recently appeared in print.[14]

VII. CONCLUSION

We have studied the forces contributing to the effective valence Z^* in electromigration. Specific models were constructed and preliminary results obtrained for the case of an impurity in the vicinity of a grain boundary (Sec. II), an impurity in the vicinity of a dislocation (Sec. III), and for an impurity in a disordered system, the latter being treated within a density matrix formalism. The nature of the local transport field in mesoscopic systems was investigated and the possibility of probing this field with an STM was considered (Sec. IV). Preliminary results, including the effects of phase-sensitivity, indicate that the STM can be a qualitative probe of the local field, except in the case of 1-d systems. Various aspects of the non-adiabatic, recoil-enhanced response of an impurity to the incident electron current were critically investigated (Sec. V), and the dynamic recoil model previously employed[3] was found to be acceptable. Portions of these investigations of recoil enhanced atomic migration were published in Physical Review Letters, October 23, 1989.

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