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2002 J. Phys.: Condens. Matter 14 L137

(http://iopscience.iop.org/0953-8984/14/6/101)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **14** (2002) L137–L140 PII: S0953-8984(02)32826-1

LETTER TO THE EDITOR

Counterbalancing forces in electromigration

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Received 17 January 2002
Published 1 February 2002
Online at stacks.iop.org/JPhysCM/14/L137

Abstract

In electromigration (EM) experiments on metallic wires, a flux of atoms can lead to motion of the centre of mass (COM) of the wire. Hence, it may be tempting to assume that the flow of current produces a net force on the wire as a whole. We point out, on the basis of known momentum-balance arguments, that the net force on a metallic wire due to a passing steady-state current is zero. This is possible, because in addition to EM driving forces, acting on scattering centres, there are counterbalancing forces, acting on the rest of the system. Drift of the COM in EM experiments occurs inevitably because the substrate keeps the crystal lattice of the wire fixed, while allowing diffusion of defects in the bulk of the wire. This drift is not evidence for a net force on the wire.

Electromigration (EM) is the directionally biased diffusion of atoms caused by the presence of an electric current. In EM experiments on pure metals it is common to see a flux of metal from the cathode toward the anode end of the wire. At the anode end one often sees the formation of hillocks due to the arrival of excess material. The centre of mass (COM) of the wire has moved toward the anode during these experiments. It may therefore be tempting to imagine that the current has produced a net body force on the wire as a whole, pushing it along the substrate.

On the basis of a self-consistent tight-binding formalism, we recently proposed that, in the presence of steady-state conduction, the sum of current-induced forces over all atoms in a system, consisting of two macroscopic electrodes connected by a metallic nanowire, vanishes [1]. A version of this zero-sum rule (ZSR) for macroscopic conductors is discussed for instance in [2, 3]. Nevertheless, in discussions with colleagues we have found that the ZSR is not universally appreciated or accepted. We have found that it divides people into two groups. Some find it obvious and trivial, while others find it highly counter-intuitive and difficult to accept, because of the notion that the flow of current in a metal should exert a net force on the metal as a whole, much like a jet of gas exerts a force on an obstacle in its way.

Here we point out that the ZSR for a macroscopic conductor follows from general momentum-balance arguments, discussed for example in [2–7]. We consider a realistic notional system, for which we attempt to state these arguments in a general way that imposes no restrictions on the structure, composition or temperature of the conductor. We have attempted to elucidate the physics behind the ZSR and to point out the crucial conditions on which it relies and which make metallic conduction different from other types of flow.

We consider a capacitor, consisting of two macroscopic electrodes, connected by a macroscopic metallic wire. The transverse size of the wire is much smaller than that of the electrodes. Electrons in the system have settled in a steady-state discharge through the wire. The wire can have local structural and compositional variations. However, there is a characteristic length scale, ξ, much less than any linear dimension of the wire, such that after averaging over this length scale, the properties of the wire are homogeneous. Within the above assumptions, we impose no restrictions on the structure, composition and temperature of the wire, or on the nature of any disorder in it. Thus, nuclei in the wire may have arbitrary identities. They may be free to vibrate thermally, or they may be frozen in arbitrary—possibly artificial—non-equilibrium positions.

Sufficiently far from each wire–electrode contact we assume that the self-consistent electronic structure in the bulk of the current-carrying wire can be described by a multiband energy–momentum dispersion relation and a one-electron occupation function. For a given structure and composition of the wire, and for a given macroscopic electron density, n, and macroscopic current density, j, this dispersion relation and occupation function, averaged over ξ, do not vary within the wire, at least to lowest order in j. An example of such a description is given by the linearized Boltzmann equation in the relaxation-time approximation [8].

Consider a macroscopic volume, V, in the bulk of the wire, far from either wire–electrode contact. All linear dimensions of V are much larger than ξ. We assume *a priori* that the acceleration of V as a whole is zero. We will now prove the ZSR by arguing that no net external force on V is needed to achieve this.

By the requirement of macroscopic charge neutrality in the bulk, n cannot vary macroscopically over the surface of V. By the requirement of continuity of current, j cannot vary macroscopically over the surface of V. Hence, the electronic band structure and occupation function, discussed above, do not vary macroscopically over the surface of V. It follows that there is no net electron momentum flux into V. Therefore, the total force on all electrons in V, F_e, vanishes.

There are three contributions to F_e. First, all charges external to V create a field in V, E_0. Let F_{E_0e} be the total force exerted by E_0 on all electrons in V. E_0 may be a complicated quantity containing contributions from any surface charges, and from any bulk polarization charges, within the electrodes and within the wire, outside V. Second, the nuclei in V exert forces on the electrons in V. Let F_{ze} be the total force exerted by the nuclei in V on all electrons in V. Third, there are forces on electrons in V due to other electrons in V. However, these forces are pairwise and cancel. As stated above, the total force on the electrons in V vanishes, or

$$F_e = F_{E_0e} + F_{ze} = 0. \tag{1}$$

Now consider the forces on the nuclei in V. Assuming overall charge neutrality in V, and ignoring correlations between E_0 and the charge density in V, we may write $F_{E_0z} = -F_{E_0e}$, where F_{E_0z} is the total force exerted by E_0 on all nuclei in V. Next, we have the force, F_{ez}, exerted on the nuclei in V by the electrons in V, given by $F_{ez} = -F_{ze}$. Nucleus–nucleus interactions are pairwise and cancel. Let F_{ext} be the total external force, if any, acting on all nuclei in V. By assumption the acceleration of the nuclei in V as a whole is zero. Hence

$$F_z = F_{E_0z} + F_{ez} + F_{ext} = -F_e + F_{ext} = 0 \tag{2}$$

where F_z is the total force on all nuclei in V. Therefore, from equation (1)

$$F_{ext} = 0. \qquad (3)$$

Thus, no net external force on the volume V as a whole is needed to prevent it from accelerating in the presence of steady-state electrical conduction. In other words, steady-state current flow does not result in a net force on a macroscopic volume in a metallic conductor. This is the ZSR.

The ZSR relies on two essential conditions. The first, expressed by the relation $F_e = 0$ above, is that the net electron momentum flux into the volume V is zero. In a metal, this condition is ensured by macroscopic charge neutrality and continuity of current. Consider by contrast the example of a gas of non-interacting particles, fired at an array of obstacles. Some of the incoming particles are reflected back by the obstacles, delivering momentum to those obstacles. Therefore the gas momentum flux into the array will be different from the gas momentum flux out of the array. The difference, given to the obstacles, results in a net force on the obstacles as a whole. Observe, however, that in this example the concentrations of gas particles on the left and on the right of the array of obstacles will be different, the difference being proportional to the amount of reflection. This contrasts with an electron current in a metal, where macroscopic charge neutrality demands that the steady-state electron concentrations are the same macroscopically on either side of an obstacle. Similarly, the ZSR will in general not be satisfied in calculations of current-induced forces in metals that do not take account of the self-consistent redistribution of electron charge in the presence of current flow. Self-consistency is essential to ensure macroscopic charge neutrality. The second condition for the ZSR, expressed by the relation $F_{E_0 z} = -F_{E_0 e}$ above, is that any external field, acting on the electrons in V, should have an equal and opposite effect on the nuclei in V. By contrast, in the above example, the device that gives the incident gas particles their initial momentum does not exert an equal and opposite force on the obstacles.

The ZSR is possible because in addition to the EM forces on defects in a metal there are counterbalancing forces on the surrounding lattice. Subject to the above conditions of charge neutrality and continuity of current, these counterbalancing forces are such as to cancel all forces acting on sources of resistivity in the metal. These counterbalancing forces were emphasized by Landauer [5]. In Landauer's analysis, the ionic subsystem is represented by jellium, plus lattice vibrations, plus identical point defects embedded in the jellium. The lattice vibrations are ripples in the jellium, or deviations from perfect jellium, and represent the thermal motion of the atoms. Landauer analysed the forces in the presence of conduction on the various components of this model system. He concluded that the total force on all point defects in a volume V of the conductor is given by

$$F_d = -jen_0(\rho - \rho_0)V \qquad (4)$$

where n_0 and ρ_0 are the carrier density and resistivity of the pure defect-free metal, respectively, and ρ is the resistivity of the metal with the defects. If, following Landauer's analysis [5], we add to F_d the forces exerted by the conduction electrons on the phonons in V, F_p, we obtain

$$F_{d+p} = F_d + F_p = -Een_0V \qquad (5)$$

where $E = j\rho$ is the total self-consistent electric field in the metal, in the presence of current flow. F_{d+p} is the total force experienced by all sources of resistivity—point defects and phonons—in V. To find the total force on all positive charges in V, we must add to F_{d+p} the force on the jellium, $F_j = Een_0V$. Therefore, $F_{d+p+j} = F_{d+p} + F_j = 0$. This is the ZSR in the framework of Landauer's analysis. Part of the total self-consistent field E in the conductor comes from electron polarization charges around each scattering centre [5, 7]. Thus, the force on the jellium, F_j, which counterbalances the forward force F_{d+p}, comes partly from the electrons themselves [5, 7].

The significance of the counterbalancing forces in a current-carrying wire may be seen by considering what would happen without them. If we consider only the force,

F_{d+p}, on all sources of resistivity—defects plus phonons—then a light-bulb filament with a cross-sectional area of the order of $A = 0.01$ mm^2, under an applied bias $W = 200$ V, would be subjected to a force of the order of $F_{d+p} = Wen_0A \sim 10^4$ N. In other words, an additional force of that magnitude would be needed to keep the filament in place, in the presence of the bias.

The ZSR does not preclude the current-induced movement of some atoms. It stipulates only that the sum of current-induced forces on all atoms in any macroscopic region of the conductor vanishes. The atoms that move are those that experience a current-induced force and that at the same time are able to move, such as interstitials or atoms adjacent to vacancies. The current-induced force on a mobile atom introduces a bias in the activation energies for migration, which results in drift and EM [9]. As is pointed out in [2], 'EM is a relative motion': that of mobile atoms through the surrounding matrix. Current-induced forces may also be thought of in terms of a current-induced stress field. This stress field may be highly spatially inhomogeneous locally, resulting in net forces on individual atoms. However, this stress field has zero net divergence over macroscopic volumes of the conductor, resulting in zero net force over such volumes.

How the COM of a metallic conductor actually moves during EM depends on the details of the experiment. For a metallic island connected to light flexible wires in free space, in the absence of any other influences, the ZSR rule suggests that conduction through the island will result in zero net acceleration of the island. Diffusion of mobile defects and EM may still occur, resulting in mass transport within the island and possibly also in an overall change in the shape and geometry of the island. However, any such current-driven deformation of the island will occur without acceleration of its COM. For a metallic wire attached to a rigid substrate, the substrate keeps the crystal lattice of the wire fixed, while allowing diffusion of defects through the lattice. This will result in a drift of the COM. For directional diffusion of defects in a lattice bonded to a rigid substrate, the COM will drift, whatever the driving force for diffusion, and whether or not the ZSR is satisfied. Such drift does not contradict the ZSR.

We wish to thank Peter Gumbsch, Reiner Moenig and Cynthia Volkert for lively discussion. We are grateful to Mike Finnis for invaluable comments. JH thanks the Leverhulme Trust for support in the initial stages of this work under grant number F/749/C. TNT thanks the EPSRC and Queen's University of Belfast for support.

References

[1] Todorov T N, Hoekstra J and Sutton A P 2000 *Phil. Mag.* B **80** 421
[2] Schaich W L 1975 *Phys. Rev.* B **13** 3350
[3] Schaich W L 1975 *Phys. Rev.* B **13** 3360
[4] Das A K and Peierls R 1975 *J. Phys. C: Solid State Phys.* **8** 3348
[5] Landauer R 1975 *J. Phys. C: Solid State Phys.* **8** L389
[6] Sham L J 1975 *Phys. Rev.* B **12** 3142
[7] Sorbello R S 1998 *Solid State Physics* vol 51 (New York: Academic) p 159
[8] Ziman J M 1972 *Principles of the Theory of Solids* (Cambridge: Cambridge University Press) ch 7
[9] Hoekstra J, Sutton A P, Todorov T N and Horsfield A P 2000 *Phys. Rev.* B **62** 8568