Electromigration-induced soliton propagation on metal surfaces

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It is demonstrated that under certain conditions, solitons can propagate on the surface of a current-carrying metal thin film. The equation of motion for small amplitude, long waves is the Korteweg–de Vries equation in the limit of high applied currents. The solitons are protrusions whose velocity decreases linearly with amplitude and that propagate in the direction of the applied electric field. [S1063-651X(99)06710-0]

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I. INTRODUCTION

The motion of the free surface of an incompressible fluid has been the subject of much research, from the 19th century to the present day. Of the many fascinating phenomena that have been investigated, soliton propagation is certainly among the most intriguing [1].

Solitons were first observed in 1834 by John Scott Russell on the surface of a narrow canal filled with water [3]. It was not until 1895, however, that it was demonstrated that solitons are solutions to the Korteweg–de Vries (KdV) equation, the equation of motion for small amplitude, long gravity waves [4].

Although it is not yet widely appreciated, there are nontrivial *electrical* free boundary problems. When an electrical current passes through a piece of solid metal, collisions between the conduction electrons and the metal atoms at the surface lead to drift of these atoms. This phenomenon, which is known as surface electromigration (SEM), can cause a solid metal surface to move and deform [5–15]. The free surface of a metal therefore moves in response to the electrical current flowing through it, in much the same way that flow in the bulk of a fluid affects the motion of its surface. However, the analogy is not perfect — the boundary conditions are very different in the two problems.

A natural question to ask is whether solitons can propagate at the free surface of a current-carrying metal thin film. Numerical studies have suggested that the answer to this question is affirmative [9,12,13]. However, these studies did not show conclusively that solitons propagate, or how their velocity varies with amplitude.

In this paper, I will demonstrate that under certain conditions, solitons do indeed propagate on the surface of a current-carrying metal thin film. The equation of motion for the surface height is the KdV equation in the limit of small film thickness, slowly varying topography, and high applied currents. The solitons are protrusions that propagate in the direction of the applied electric field. Their velocity *decreases* linearly with amplitude; in contrast, the velocity of a soliton in a narrow channel of water increases with amplitude.

It is worth mentioning that SEM is not just of academic interest: It can lead to the electrical failure of a current-carrying metal line, and consequently is an important factor limiting the reliability of integrated circuits. For applied currents in excess of a critical value, SEM causes a small perturbation at the edge of a metal strip to become a slit-shaped void [14–17]. This slit propagates across the line, and causes electrical failure when its tip contacts the opposite edge of the strip.

II. EQUATIONS OF MOTION

Consider a metal film of thickness h_0 deposited on the plane surface of an insulating substrate. We take the z axis to be normal to the substrate surface and locate the origin in this plane. A constant current flows through the film in the x direction, and the electric field within the metal is $E_0\hat{x}$.

Now suppose that the upper surface of the film is perturbed (Fig. 1). Let the outward-pointing unit normal to this surface be $\hat{n}$. For simplicity, we shall restrict our attention to perturbations whose form does not depend upon y, so that the height of the film's surface above the substrate h depends only on x and t. The upper film surface will evolve in the course of time due to the effects of SEM and surface self-diffusion. We assume that the current flowing through the film is held fixed.

Clearly, the problem is two-dimensional (2D), and the dependence of all quantities on y will therefore be suppressed. The electrical potential $\Phi = \Phi(x,z,t)$ satisfies the 2D Laplace equation

$$\nabla^2\Phi = 0, \tag{1}$$

and is subject to the boundary condition $\hat{n}\cdot\vec{\nabla}\Phi = 0$ on the upper surface and $\hat{z}\cdot\vec{\nabla}\Phi = 0$ on the lower. More explicitly, we have

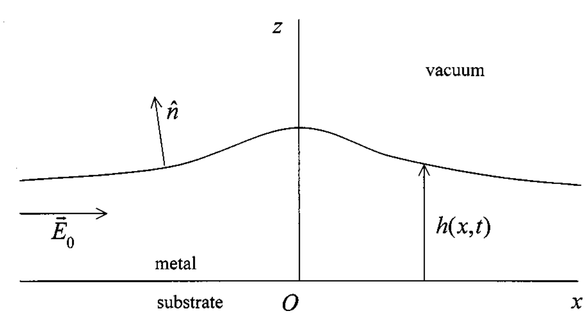

FIG. 1. The current-carrying metal thin film. The height of the free surface above the substrate, h, depends only on x and t. The outward-pointing unit normal to the free surface is $\hat{n}$, and the electric field far from the perturbation is $\vec{E}_0$.

$$\Phi_z(x,h,t)=h_x\Phi_x(x,h,t), \tag{2}$$

and

$$\Phi_z(x,0,t)=0, \tag{3}$$

where $f_x \equiv \partial f/\partial x$ and so forth. If the initial perturbation is localized, we will also have

$$\Phi(x,z,t)\to -E_0 x, \tag{4}$$

for $x\to\pm\infty$ and $0\leqslant z\leqslant h_0$.

We assume that the mobility of the metal atoms is negligible at the metal-insulator interface, so that the form of that interface remains planar for all time. Furthermore, in the interest of simplicity, we assume that the applied current is high enough that the effects of SEM are much more important than those of capillarity. The equation of motion for the metal-vacuum interface is then [9]

$$h_t=qM\frac{\partial}{\partial x}\left(\frac{1}{\sqrt{1+h_x^2}}\frac{\partial\Phi}{\partial x}\right), \tag{5}$$

where q is the effective charge of a metal ion and M, the adatom mobility, has been assumed to have negligible anisotropy. Together, Eqs. (1)–(5) completely describe the nonlinear dynamics of the film surface.

III. ASYMPTOTIC ANALYSIS

We wish to study the propagation of a localized disturbance whose amplitude is small compared to h_0, and whose width is large compared to h_0. To do so, we will use multiple scale asymptotic analysis [2]. We put $h=h_0+a\zeta$, where the constant a is a measure of the amplitude of the disturbance and $\zeta=\zeta(x,t)$ is of order unity. Let l be the characteristic width of the initial disturbance. We will study the limit in which both $\alpha\equiv a/h_0$ and $\delta\equiv h_0/l$ are small. More precisely, we shall consider the limit in which α and δ tend to zero, but α/δ^2 remains finite. It is in this limit that the effects of nonlinearity and dispersion balance, and solitons propagate.

To simplify the description of the problem, we will set $\Phi=-E_0x+\phi$, so that $\phi\to 0$ for $x\to\pm\infty$. We also introduce the dimensionless quantities $\tilde{x}\equiv x/l$, $\tilde{z}\equiv z/h_0$, $\tilde{t}\equiv(|q|ME_0/h_0 l)t$, and $\tilde{\phi}(\tilde{x},\tilde{z},\tilde{t})\equiv\phi(x,z,t)/(E_0 l)$. Eq. (1) becomes

$$\tilde{\phi}_{\tilde{z}\tilde{z}}+\delta^2\tilde{\phi}_{\tilde{x}\tilde{x}}=0, \tag{6}$$

which applies for $0\leqslant\tilde{z}\leqslant 1+\alpha\zeta(\tilde{x},\tilde{t})$ and all $\tilde{x}$. The boundary conditions are

$$\tilde{\phi}_{\tilde{z}}=0 \qquad \text{for } \tilde{z}=0, \tag{7}$$

$$\tilde{\phi}_{\tilde{z}}=\alpha\delta^2(\tilde{\phi}_{\tilde{x}}-1)\zeta_{\tilde{x}} \qquad \text{for } \tilde{z}=1+\alpha\zeta(\tilde{x},\tilde{t}), \tag{8}$$

and

$$\tilde{\phi}\to 0 \quad \text{for } 0\leqslant\tilde{z}\leqslant 1 \qquad \text{and } \tilde{x}\to\pm\infty. \tag{9}$$

Finally, the equation of motion for the free surface of the film is

$$\sigma_q\alpha\zeta_{\tilde{t}}=\frac{\partial}{\partial\tilde{x}}\left(\frac{\tilde{\phi}_{\tilde{x}}-1}{\sqrt{1+\alpha^2\delta^2\zeta_{\tilde{x}}^2}}\right) \quad \text{for } \tilde{z}=1+\alpha\zeta(\tilde{x},\tilde{t}). \tag{10}$$

Here $\sigma_q\equiv q/|q|$.

We next introduce the scaled variables

$$\xi\equiv\frac{\alpha^{1/2}}{\delta}(\tilde{x}+\sigma_q\tilde{t}), \tag{11}$$

$$\tau\equiv\frac{\alpha^{3/2}}{\delta}\tilde{t}, \tag{12}$$

and

$$\psi\equiv\frac{\alpha^{1/2}}{\delta}\tilde{\phi}. \tag{13}$$

(ξ,τ) is a moving coordinate system that translates with velocity $v_0\equiv -qME_0/h_0$ relative to the laboratory frame. v_0 is the velocity of surface waves in the limit of vanishing amplitude and wave vector [9].

For convenience, we drop the tilde on z. Laplace's equation becomes

$$\psi_{zz}+\alpha\psi_{\xi\xi}=0, \tag{14}$$

and this applies for $0\leqslant z\leqslant 1+\alpha\zeta(\xi,\tau)$ and all ξ. In terms of the scaled variables, Eqs. (7)–(10) are

$$\psi_z=0 \qquad \text{for} \qquad z=0, \tag{15}$$

$$\psi_z=\alpha^2(\psi_\xi-1)\zeta_\xi \qquad \text{for} \qquad z=1+\alpha\zeta(\xi,\tau), \tag{16}$$

$$\psi\to 0 \quad \text{for } 0\leqslant z\leqslant 1 \qquad \text{and} \qquad \xi\to\pm\infty, \tag{17}$$

and

$$\alpha\zeta_\xi+\sigma_q\alpha^2\zeta_\tau=\frac{\partial}{\partial\xi}\left(\frac{\psi_\xi-1}{\sqrt{1+\alpha^3\zeta_\xi^2}}\right) \qquad \text{for} \quad z=1+\alpha\zeta(\xi,\tau). \tag{18}$$

One advantage of introducing the scaled variables is now manifest: δ does not appear explicitly in Eqs. (14)–(18).

We shall now begin our analysis of the small α limit. We assume that for small α and fixed ξ and τ, there is a solution with

$$\psi=\sum_{n=0}^{\infty}\alpha^n\psi_n(\xi,\tau,z) \tag{19}$$

and

$$\zeta=\sum_{n=0}^{\infty}\alpha^n\zeta_n(\xi,\tau,z), \tag{20}$$

where the ψ_n's and ζ_n's are independent of α.

We next insert the expansions (19) and (20) into Eqs. (14)–(18) and equate terms of the same order in α. The goal will be to find a closed partial differential equation for ζ_0. We will need to consider terms up to order α^3. To prepare for this task, we note that to third order in α, Eq. (16) is

$$\psi_z+\alpha\zeta\psi_{zz}+\frac{1}{2}\alpha^2\zeta^2\psi_{zzz}+\frac{1}{6}\alpha^3\zeta^3\psi_{zzzz}$$
$$=\alpha^2(\psi_\xi+\alpha\zeta\psi_{\xi z}-1)\zeta_\xi. \quad (21)$$

This result holds for $z=1$. To second order in α, Eq. (18) implies that for $z=1$

$$\alpha\zeta_\xi+\sigma_q\alpha^2\zeta_\tau=\psi_{\xi\xi}+\alpha(\zeta_0+\alpha\zeta_1)(\psi_{0\xi\xi z}+\alpha\psi_{1\xi\xi z})$$
$$+\frac{1}{2}\alpha^2\zeta_0^2\psi_{0\xi\xi zz}. \quad (22)$$

We begin by working to zeroth order in α. To this order, Eq. (14) becomes $\psi_{0zz}=0$ for $0\leqslant z\leqslant 1$. This implies that ψ_{0z} does not depend on z. Applying Eq. (15), we see that in fact $\psi_{0z}=0$ for all ξ and τ. We conclude that ψ_0 depends only on ξ and τ, and we write

$$\psi_0=\theta_0(\xi,\tau). \quad (23)$$

The boundary condition at the free surface of the film gives no new information to zeroth order in α, as is readily seen from Eq. (21). Lastly, Eq. (23) shows that

$$\theta_{0\xi\xi}=0. \quad (24)$$

To first order in α, we find that ψ_1 is independent of z. We shall write

$$\psi_1=\theta_1(\xi,\tau). \quad (25)$$

Equation (21) again yields no new information. Using the fact that $\psi_{0z}=0$, we see that the equation of motion (22) is to first order

$$\zeta_{0\xi}=\theta_{1\xi\xi}. \quad (26)$$

Our next task will be to write out the equations of motion to order α^2. Equation (14) shows that $\psi_{2zz}+\psi_{1\xi\xi}=0$ for $0\leqslant z\leqslant 1$, and hence $\psi_{2zz}=-\theta_{1\xi\xi}$. Integrating this with respect to z and using the boundary condition at the metal-insulator interface (15), we have $\psi_{2z}=-\theta_{1\xi\xi}z$. Integrating once again, we obtain

$$\psi_2=\theta_2-\frac{1}{2}\theta_{1\xi\xi}z^2, \quad (27)$$

where θ_2 depends only on ξ and τ. Equation (21) yields new information as well: specifically, $\psi_{2z}=(\psi_{0\xi}-1)\zeta_{0\xi}$ for $z=1$. Inserting Eqs. (23) and (27) into this result, we see that

$$\zeta_{0\xi}=\frac{\theta_{1\xi\xi}}{1-\theta_{0\xi}}. \quad (28)$$

We wish to find a nontrivial solution for ζ_0, i.e., one that depends on ξ. $\theta_{1\xi\xi}$ must therefore be nonzero. Comparing Eqs. (26) and (28), we see that for a nontrivial solution, we must insist that

$$\theta_{0\xi}=0. \quad (29)$$

Equation (22) gives $\zeta_{1\xi}+\sigma_q\zeta_{0\tau}=\psi_{2\xi\xi}$ for $z=1$. Using Eqs. (26) and (27) in this result, we have

$$\sigma_q\zeta_{0\tau}+\frac{1}{2}\zeta_{0\xi\xi\xi}=\theta_{2\xi\xi}-\zeta_{1\xi}. \quad (30)$$

Equating terms of order α^3 in Eq. (14) yields $\psi_{3zz}+\psi_{2\xi\xi}=0$ for $0\leqslant z\leqslant 1$. Integrating this twice with respect to z and applying Eqs. (15) and (27), we find that

$$\psi_3=\theta_3-\frac{1}{2}\theta_{2\xi\xi}z^2+\frac{1}{24}\theta_{1\xi\xi\xi\xi}z^4, \quad (31)$$

where $0\leqslant z\leqslant 1$ and $\theta_3=\theta_3(\xi,\tau)$. We next equate terms of third order in Eq. (21). We obtain

$$\psi_{3z}+\zeta_0\psi_{2zz}=\psi_{1\xi}\zeta_{0\xi}+(\psi_{0\xi}-1)\zeta_{1\xi} \quad (32)$$

for $z=1$. This can be simplified using Eqs. (25), (27), (29), and (31). The result is

$$\theta_{2\xi\xi}-\zeta_{1\xi}=\frac{1}{6}\theta_{1\xi\xi\xi\xi}-\zeta_0\theta_{1\xi\xi}-\theta_{1\xi}\zeta_{0\xi}. \quad (33)$$

Integrating Eq. (26) with respect to ξ yields $\theta_{1\xi}=\zeta_0+F$, where F is a function of τ. Recall that we have assumed that the disturbance is localized. This means that $\theta_{1\xi}$ and ζ_0 should both tend to zero when ξ is large, and hence $F(\tau)=0$ for all τ. Equation (33) may therefore be rewritten as follows:

$$\theta_{2\xi\xi}-\zeta_{1\xi}=\frac{1}{6}\zeta_{0\xi\xi\xi}-2\zeta_0\zeta_{0\xi}. \quad (34)$$

Comparing this with Eq. (30), we have

$$\sigma_q\zeta_{0\tau}+\frac{1}{3}\zeta_{0\xi\xi\xi}+2\zeta_0\zeta_{0\xi}=0. \quad (35)$$

Equation (35) is the KdV equation, albeit in a nonstandard form. Setting $u=-\zeta_0$, $T=\tau/3$, and $X=\sigma_q\xi$, we obtain

$$u_T-6uu_X+u_{XXX}=0, \quad (36)$$

the standard form of the KdV equation. This has the solitary wave solution

$$u(X,T)=-\frac{1}{2}c\,\mathrm{sech}^2\left[\frac{1}{2}c^{1/2}(X-cT)\right], \quad (37)$$

where c is a positive constant. In terms of the original, unscaled variables, Eq. (37) is

$$h=h_0+\frac{1}{2}A\,\mathrm{sech}^2\left[\frac{1}{2}\sqrt{\frac{A}{h_0^3}}(x-vt)\right]. \quad (38)$$

Here $A\equiv ac$ is the amplitude of the soliton and

$$v\equiv v_0\left(1-\frac{A}{3h_0}\right) \quad (39)$$

is its velocity. Note that the velocity of the soliton decreases with amplitude, in contrast to the behavior of solitary waves in shallow water [2]. The width of the soliton, $w\equiv 2\sqrt{h_0^3/A}$, also decreases with the amplitude.

The amplitude A is positive, and so the solitons are protrusions. For metals, the effective charge q is negative, which means that a soliton will propagate to the right, in the direction of the applied field (Fig. 1). The reason for this is readily apparent. The electric field on the metal surface has reduced magnitude in the vicinity of the soliton. Therefore, the wind force will deposit atoms on the right side of the protrusion and remove them from the left. The net result is a soliton that propagates to the right. In contrast, solitons can propagate in both directions in a shallow channel of water.

IV. DISCUSSION

In our formulation of the problem, we made two key simplifications: we took the adatom mobility M to be isotropic, and assumed that the electric field is strong enough that the effects of surface self-diffusion are negligible compared to those of surface electromigration. We will now discuss these simplifications in greater detail.

We begin by writing Eq. (35) in terms of the unscaled variables x and t. Let $u \equiv h - h_0$. Equation (35) may be written

$$u_t = -v_0 u_x + \frac{1}{3} v_0 h_0^2 u_{xxx} + 2\frac{v_0}{h_0} u u_x . \tag{40}$$

How large must the electric field be for the effects of surface self-diffusion to be negligible? If the effects of surface self-diffusion are taken into account, a term $-Bu_{xxxx}$ must be added to the right-hand side of Eq. (40). Here

$$B \equiv \frac{D\gamma\Omega^2\nu}{k_B T}, \tag{41}$$

where D is the surface self-diffusivity, γ is the surface tension, Ω is the atomic volume, and ν is the number of mobile adatoms per unit surface area [18]. We require that the effects of surface self-diffusion be small compared to those of the dispersive and nonlinear terms. A straightforward scaling analysis reveals that this will be so if

$$l_E^2 \ll h_0 l, \tag{42}$$

where $l_E \equiv (\gamma\Omega/qE_0)^{1/2}$ is a length characterizing the relative importance of SEM and capillarity. For the remainder of our discussion, we assume that Eq. (42) is valid and neglect surface self-diffusion.

The adatom mobility M is anisotropic for any real single crystal metal film. If the mobility is not isotropic, then M depends on h_x and Eq. (5) must be replaced by

$$h_t = q\frac{\partial}{\partial x}\left(\frac{M(h_x)}{\sqrt{1+h_x^2}}\frac{\partial\Phi}{\partial x}\right). \tag{43}$$

The anisotropy alters the equation of motion of the surface to *linear* order [5]; for slowly varying topography, the linearized equation of motion is

$$u_t = -v_0 u_x - qM'(0)E_0 u_{xx} + \frac{1}{3} v_0 h_0^2 u_{xxx} . \tag{44}$$

Incorporating the leading order nonlinearity, we have

$$u_t = -v_0 u_x - qM'(0)E_0 u_{xx} + \frac{1}{3} v_0 h_0^2 u_{xxx} + 2\frac{v_0}{h_0} u u_x . \tag{45}$$

If $qM'(0)E_0 > 0$, the second term on the right-hand side of Eq. (45) produces a linear instability in the surface, as first recognized by Krug and Dobbs [5]. If $qM'(0)E_0$ is negative, on the other hand, any surface disturbance will decay in the course of time. In both cases, solitons will not propagate.

Does this mean that the result of our analysis is physically irrelevant? Fortunately, the answer to this question is no — solitons will propagate if $M'(0)=0$, and $M'(0)$ vanishes for a singular surface of a single crystal film. To establish that solitons propagate if $M'(0)=0$, we must show that the leading order nonlinear term coming from the mobility anisotropy is negligible compared to the dispersive and nonlinear effects of SEM. Setting $M(h_x) = M(0) + \frac{1}{2} M''(0) h_x^2$ in Eq. (43), we obtain

$$\begin{aligned} u_t &= qM(0)\frac{\partial}{\partial x}\left(\frac{1}{\sqrt{1+u_x^2}}\frac{\partial\Phi}{\partial x}\right) \\ &\quad + \frac{1}{2} qM''(0)\frac{\partial}{\partial x}\left(\frac{u_x^2}{\sqrt{1+u_x^2}}\frac{\partial\Phi}{\partial x}\right). \end{aligned} \tag{46}$$

To leading order, this reduces to

$$u_t = qM(0)\frac{\partial}{\partial x}\left(\frac{1}{\sqrt{1+u_x^2}}\frac{\partial\Phi}{\partial x}\right) - qM''(0)E_0 u_x u_{xx} . \tag{47}$$

The equation of motion (40) therefore becomes

$$u_t = -v_0 u_x + \frac{1}{3} v_0 h_0^2 u_{xxx} + 2\frac{v_0}{h_0} u u_x - qM''(0)E_0 u_x u_{xx} . \tag{48}$$

A straightforward scaling analysis shows that the final term on the right-hand side of Eq. (48) is smaller by a factor of α than the preceding two terms, and this is what we set out to show.

Electromigration-induced soliton propagation has not yet been observed experimentally. For it to be observed, a single crystal metal thin film with a singular surface should be prepared. Once the surface has been perturbed, a high electric field should be applied. The solitons will be protrusions that propagate in the direction of the applied field. Suppose the applied field points to the right, as in Fig. 1. As we have seen, small amplitude solitons move faster than large amplitude solitons. Thus, it should be possible to watch a small amplitude soliton overtake a large amplitude soliton to its right. After the collision has taken place, the two solitons will emerge with their identities intact, with the smaller soliton to the right of the larger. A phase shift will be the only aftereffect of the collision [2].

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[1] For an excellent introduction to the topic, see Ref. [2].
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