Islands in the Stream: Complex Shape Evolution Driven by Surface Electromigration

P. Kuhn, University of Duisburg-Essen
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Supported by DFG within SFB 616 Energy Dissipation at Surfaces & SFB 611 Singular phenomena and scaling in mathematical models

\(^1\)cond-mat/0405068 & 0410745
Island in the Straits:

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\footnote{cond-mat/0405068 & 0410745}
Surface Electromigration

Electromigration force:
\[ F = eZ^*E \]

- relation to surface resistance and electronic friction
- dominant failure mechanism in integrated circuits

\( i = -nve \)

\( Z^* \): effective valence
Surface Electromigration

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**General goal:** To bridge the gap between atomistic processes and large scale morphological evolution through the study of simple step and island configurations on single crystal surfaces
Surface Electromigration

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Model problems:

- electromigration-induced step bunching
- current effects on step fluctuations
- electromigration of single layer islands
Surface Electromigration

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Model problems:
- electromigration-induced step bunching \( \rightarrow \) M. Uwaha, J. Weeks (today)
- current effects on step fluctuations \( \rightarrow \) E. Williams (yesterday)
- electromigration of single layer islands \( \rightarrow \) this talk
Continuum Model of Shape Evolution

- mass transport restricted to the one-dimensional interface
- anisotropic mobility and stiffness

- normal edge velocity $v_n$ satisfies

$$v_n + \frac{\partial j}{\partial s} = 0, \quad j = \sigma(\theta) \left[ F_t - \frac{\partial}{\partial s} \tilde{\gamma}(\theta) \kappa \right]$$

$s$: arc length \quad $\theta$: edge orientation \quad $\kappa$: edge curvature

$\sigma(\theta)$: adatom mobility \quad $\tilde{\gamma}(\theta)$: step stiffness \quad $F_t$: tangential force

- electromigration dominates on length scales $\gg l_E = \sqrt{\tilde{\gamma}/|F|}$

- Numerical methods: Finite differences & adaptive finite elements
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**Islands vs. Voids**

- **Local model:** $F_t = F_0 \cos(\theta + \phi)$  \( \phi \): field direction
  - single layer islands (Pierre-Louis & Einstein 2000)
  - dislocation loops (Suo 1994)

- **Nonlocal model:** $F_t = -\frac{\partial U}{\partial s}$ with $\nabla^2 U_{\text{outside}} = U_{\text{inside}} = 0$
  - insulating voids in metallic thin films
  (Kraft & Arzt, Gungor & Maroudas, Mahadevan & Bradley, Schimschak & JK...)

- Interpolation by general conductivity ratio $\rho = \frac{\Sigma_{\text{inside}}}{\Sigma_{\text{outside}}} \in [0, 1]$
Results for the isotropic case

- The circle is a stationary solution for any $\rho$ (Ho, 1970)

- Linear instability at critical radius $R_c^{(1)} = \hat{R}_c^{(1)} l_E$ for $\rho > 0$ (Wang, Suo, Hao 1996)

- Nonlinear instability for $\rho = 0$ (Schimschak & JK, 1998)

- No non-circular stationary shapes for $\rho = 0$ (Cummings, Richardson, Ben Amar 2001)

- $\rho = 1$: Non-circular stationary shapes are stable for

$$\hat{R}_c^{(1)} \approx 3.26 < R/l_E < \hat{R}_c^{(2)} \approx 6.2$$
Non-circular stationary shapes

- Dimensionless initial radius $R_0 = R/l_E = 3.3, 4, 5, 6$

- Shapes approach a finger solution of width $W \approx 4.8l_E$
  (Suo, Wang, Yang 1994)
- Dimensionless radius $R_0 = R/l_E = 7$

- Breakup mediated by outgrowth of finger
Void breakup


- Splitoff of **circular** void, no finger solution
Island breakup in kinetic Monte Carlo simulations

Anisotropic stationary shapes without capillarity

- Island moves along $x$-axis

- Parametrization: $x = x(\theta), y = y(\theta)$
  $$\frac{dy}{dx} = -\tan(\theta)$$

- Stationarity condition: $v_n = V \sin(\theta) \Rightarrow V_y = j + \text{const.}$ (Suo 1994)

- In the absence of capillarity ($\tilde{\gamma} = 0$) this implies
  $$y(\theta) = \frac{F}{V} \sigma(\theta) \cos(\theta + \phi), \quad x(\theta) = -\int_0^\theta d\theta' \frac{dy}{d\theta'} \cot(\theta')$$

- Mobility model: $\sigma(\theta) = \sigma_0 \left[ 1 + S \cos^2[n(\theta + \alpha)/2] \right]$ \quad $S$: Anisotropy strength
  $n$: Number of symmetry axes
  $\alpha$: Orientation of symmetry axes
Conditions on physical shapes:

(i) \( x(\theta) \) finite \( \Rightarrow dy/d\theta = 0 \) at \( \theta = 0 \) and \( \pi \)

(ii) no self-intersections \( \Rightarrow dy/d\theta \neq 0 \) for \( \theta \neq 0, \pi \)

(iii) closed contour: \( x(\theta + 2\pi) = x(\theta) \Rightarrow \tan(n\alpha)\tan(\phi) = n \) for odd \( n \)

Consequences:

- No stationary shapes for odd \( n \)!

- For even \( n \) smooth stationary shapes exist in a range \( 0 < S < S_c \) of anisotropy strengths

- Condition (i) selects direction of island motion which is generally different from the direction of the field
Stationary shapes without capillarity for $n = 6$

- Direction of motion may vary discontinuously with $\alpha - \phi$
Anisotropic stationary shapes with capillarity

\[ R_0 = 2.5 \]

\[ \sigma(\theta) = \sigma_0 \{1 + S \cos^2[n\theta/2]\}, \text{isotropic stiffness} \]

\[ R_0: \text{Dimensionless radius of a circle of the same area} \]
Obliquely moving stationary shapes \((n=6, S=2)\)

\[
R_0 = 2.4 \quad R_0 = 2.7 \quad R_0 = 3.0
\]

- Spontaneous breaking of symmetry w.r.t. field & anisotropy direction
Angle of motion as an order parameter \((S = 2)\)

SS: straight stationary
OS: oblique stationary
OO: oblique oscillatory
Oblique oscillatory motion

* Dimensionless radius $R_0 = 4$, anisotropy strength $S = 1$

* Upper edge is linearly stable, lower edge linearly unstable
Zig-zag motion

$R_0 = 3.5, S = 0.5$

$R_0 = 3.5, S = 1$
Regular and irregular oscillations of the island perimeter

characteristic time scale: \( t_E = l_E^4 / \sigma_{\max} \tilde{\gamma} \)
Complex oscillatory motion

$S = 3, R_0 = 8$
Selected facets and the origin of oscillations

- Large islands are composed of selected facets which are stationary in the substrate frame. Oscillations arise because islands slide past the static facets.

- Facets are constant current solutions of the evolution equation:

\[ j = j^* \Rightarrow \tilde{\gamma} \frac{d^2}{ds^2} \theta(s) = -\frac{j^*}{\sigma(\theta)} + F_0 \cos(\theta) \equiv -V'(\theta) \]

- Facet orientations are degenerate maxima of the “potential” \( V(\theta) \)

- For \( n = 6, \alpha = 0 \) there are four selected orientations, out of which three are needed to form a closed island:
A tentative phase diagram

- **bu**: island breakup
- **co**: complex oscillatory
- **oo**: oblique oscillatory
- **zz**: zig-zag
- **os**: oblique stationary
- **ss**: straight stationary
Divergence of the oscillation period at the oo \( \rightarrow \) os transition

- \( N \): Number of discretization points
- Best fit: \( \tau \sim (R_0 - R_c)^{-2.5} \)
Oscillatory behavior in void electromigration


- Propagation of edge voids with crystal anisotropy

- Onset of oscillations at a critical void size

- Divergence of oscillation period at onset
Experimental considerations: Islands on Cu(100)

- Electromigration force on a step atom: $400 \text{ eV/cm}$ at $i = 10^7 \text{ A/cm}^2$
  

- Step stiffness $\tilde{\gamma} \approx 0.13 \text{ eV/atom}$ for kinked steps
  

  $\Rightarrow \ l_E \approx 25 - 100 \text{ nm}$

- Characteristic time scale from step fluctuation kinetics
  

  $\Rightarrow \ t_E = \frac{l_E^4}{\sigma_{\text{max}} \tilde{\gamma}} \approx 1 \text{ s} \text{ at } 300 \text{ K}$
Outlook

- Nature of bifurcations (low-dimensional truncation)?

- Oscillatory behavior in kinetic Monte Carlo simulations?

- Nonlinear behavior in the kinetic regimes involving mass exchange with the terrace?