Thin solid films: PDE models of surface instabilities and surface dynamics

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Modeling formation of pits in the Si thin film on the quartz or sapphire substrate

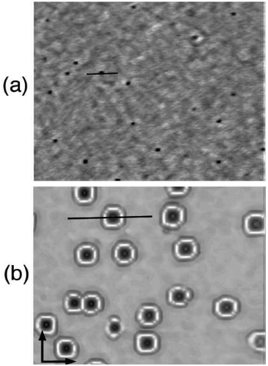
Semiconductor Si thin films form the basis of most micro and nanoelectronic devices, such as LEDs, themal actuators, transistors and optical waveguides; they are also used in solar cells.

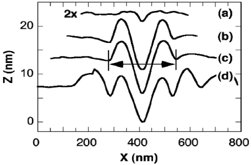
All such devices operate at high T: about $1000^{\circ} - 1100^{\circ}$C, which is below the melting T of silicon: 1414°C.

High T causes **surface diffusion of atoms**, which results in changes to the film height; that is, $h = h(x, t)$.

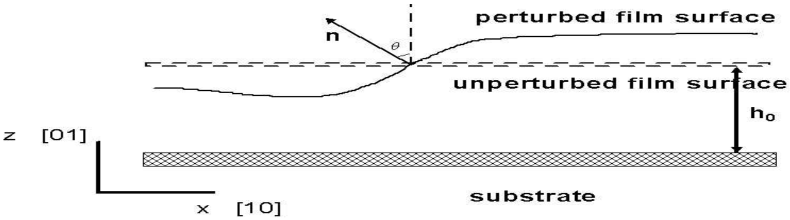
Atomic Force Microscope images of the Si film surface (top-down view) one hour after raising the temperature to 550 C.

(a) $h_0 = 5$ nm; (b) $h_0 = 20$ nm. (from [5]). Pits form in the film !





View of the film surface from the side



Evolution Partial Differential Equation for $h(x,t)$

The nonlinear, 6th-order evolution PDE for the height of a thin film:

$$\begin{aligned} h_t &= B\frac{\partial}{\partial x}\left[(\cos\theta)\frac{\partial}{\partial x}\left(\mathcal{M}_w+\mathcal{M}_\gamma\right)\right] \\ &\equiv F\left(h(x,t), h_x, h_{xx}, ..., h_{xxxxxx}\right), \quad \text{where} \end{aligned}$$

$$B = const.\text{ is Mullins' number;} \quad \cos\theta = (1+h_x^2)^{-1/2},$$

$$\mathcal{M}_w = \frac{\partial\gamma(h,\theta)}{\partial h}\cos\theta = \left(\gamma^{(f)}(\theta) - G\right)e^{-h}\cos\theta,$$

$$\mathcal{M}_\gamma = \left(\gamma(h,\theta)+\gamma_{\theta\theta}(h,\theta)\right)\kappa, \quad \kappa = -h_{xx}/(1+h_x^2)^{3/2},$$

$$\gamma(h,\theta) = \gamma^{(f)}(\theta) + \left(G-\gamma^{(f)}(\theta)\right)e^{-h},$$

$$\gamma^{(f)}(\theta) = 1 + A\cos 4\theta + \frac{\Delta}{2}\kappa^2, \quad \cos 4\theta = f\left(\cos\theta\right) = 8\cos^4\theta - 8\cos^2\theta + 1.$$

$\mathcal{M}_w$ and $\mathcal{M}_\gamma$ are the *chemical potentials*

Use the 6th-order nonlinear evolution PDE $h_t = F(h, h_x, h_{xx}, \dots)$ as derived, or the parametric re-formulation to account for non-graph pit shapes

The initial condition:

$$h(x,0) = 1 - d \exp\left[-\left(\frac{x-5}{w}\right)^2\right], \quad 0 \le x \le 10$$

$d = 0.5$ (shallow pit) AND one of the following:

$w = 0.15$ (narrow pit), or

$w = 1$ (intermediate pit), or

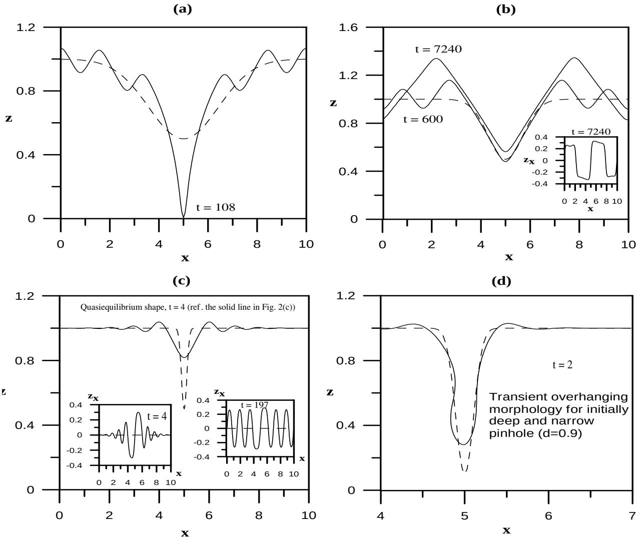
$w = 2$ (wide pit)

Periodic b.c.'s at $x = 0$ and $x = 10$

$$G = 0.5, \quad A = 1/12, \quad B = 3.57 \times 10^{-3}$$

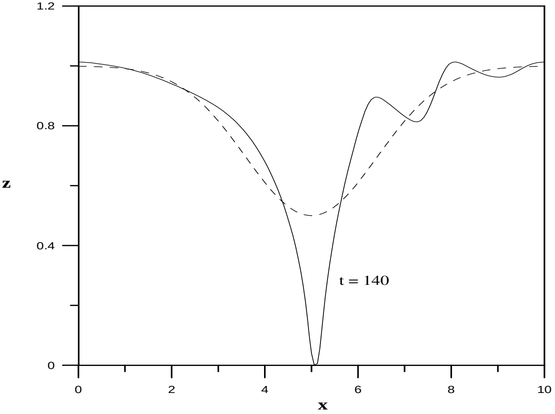
The numerical method: Method of Lines, using a stiff ODE solver

The pit shapes



(a): $w = 2$, (b): $w = 1$, (c): $w = 0.15$

Rotate sample, expose different crystallographic orientation:
$\gamma^{(f)}(\theta) = 1 + A\cos 4(\theta + \beta) + \frac{\Delta}{2}\kappa^2$



$w = 2,\ \beta = 10^\circ$

References

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