

Morphological stability of strained thin solid films

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Strained thin solid films are nowadays widely integrated in many applicative fields to boost the devices' performances. In photonics and nanoelectronics, strained semiconductors are currently integrated to tune their optical and electronic properties. However, during high temperature annealing, the strain state of the integrated materials can largely evolved leading to a loss of the integrity of the strained thin semiconductor solid films. One of the detrimental physical phenomena which can occurs is surface diffusion driven dewetting [1] leading to the agglomeration of the considered thin solid films. In this paper we will first review the numerical methodology adopted to simulate surface diffusion including strain impact. Then an enrichment of the well-known Asaro-Tiller-Grinfeld stability domain will be proposed: a stable oscillatory regime where surface oscillation laterally propagates but no longer grows in amplitude will be demonstrated. Impact of strain level and of the relative film-to-substrate elastic stiffness will be illustrated.

To track morphological evolution through surface diffusion, surface chemical potential is the first ingredient to compute in order to evaluate surface fluxes according to Nernst-Einstein equation. Surface potential formulation on a discretized surface was proposed by considering local infinitesimal matter accretion as a thought experiment. This leads to an analytical convenient formulation including both capillary and elastic contributions. The adopted formulations for the capillary and elastic contribution to the Surface chemical potential are [2-3]:

$$\mu_{cap} = \mu_{cap}^0 + 2\gamma\Omega_0 \frac{\sin(\theta_l) - \sin(\theta_r)}{\frac{b_l}{1+Tr[\varepsilon_l]} + \frac{b_r}{1+Tr[\varepsilon_r]}}, \quad \mu_{el} = \mu_{el}^0 + 2\Omega_0 \frac{\omega_l \cdot b_l + \omega_r \cdot b_r}{\frac{b_l}{1+Tr[\varepsilon_l]} + \frac{b_r}{1+Tr[\varepsilon_r]}}$$

where γ , Ω^0 and μ^0 are surface energy, unstrained atomic volume and reference surface chemical potential for unstrained and flat surface. Such a formulation can be easily generalized to take into account surface energy anisotropy. This discrete formulation can also be applied on the triple line (atmosphere/solid/solid coincident line) to treat dewetting of solid patterns from a substrate [2]. Obviously such a formulation allows studying the stability of strained thin solid films [3] and more widely to study the dynamics of destabilization of strained thin solid films through surface diffusion.

To study the stability of strained thin solid films, a small and local perturbation is introduced at the surface as previously described in [3]. From this perturbation, the well-known Asaro-Tiller-Grinfeld instability can occur depending on strain level and film thickness [3,4]. Figure 1 illustrates the results obtained for a strained 10 nm solid film lying on a substrate which elastic stiffness varies (ρ stands for the ratio between film's thickness over substrate's thickness). In-plane strain components in the film are here initially imposed to be 1% whereas substrate stiffness is define.

When entering instability domain, the system will naturally select the wavelength for which the growth velocity is maximum as illustrated on figure 1 (red lines). Calculated selected wavelength (λ_{nm} , closed red square) is then very closed to the wavelength obtained through small perturbation theory [4] (λ_m , open red square).

Due to the local small perturbation initially defined, the growth rate v_{nm} of the developed instability is almost constant in a first time region but is significantly lower than the predicted one (v_m). This difference is explained by the fact that lateral expansion and amplitude growth of the instability occur simultaneously and largely decrease the growth rate which can reach the theoretical prediction asymptotically.

Finally when considering large substrate elastic rigidity ($\rho < 0.5$), the instability amplitude cannot exceed a certain portion of the initial film thickness as illustrated by the black dots which report the calculated value of the film thickness which remain unaffected by the surface oscillation. This particular regime in which a stable oscillatory surface with fixed amplitude is finally obtained extend the stability domain predicted by small perturbation theory.

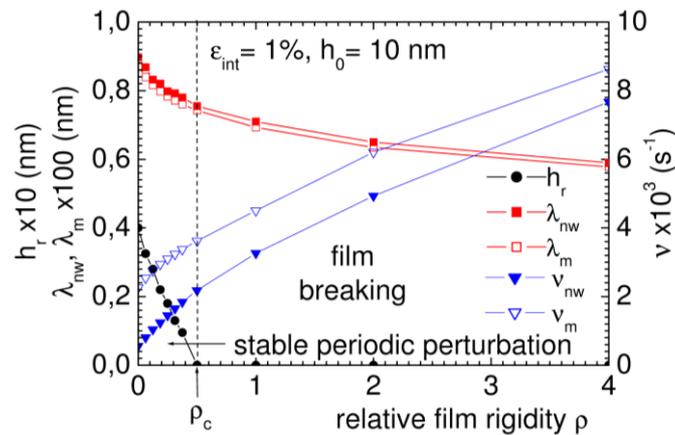


Figure 1: Selected wavelength λ , growth rate v and thickness unaffected by the surface oscillation h_r as a function of the relative film to substrate rigidity

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