Mean Curvature and Surface Diffusion Motions: Symmetries and Special Solutions

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Some physical concepts

- **A grain (crystal):** a material composed of atoms arranged on a crystalline lattice.
- **Polycrystalline materials:** materials composed of many grains, varying in size and orientation.
- **Thin films:** material layers with thickness ranging from nanometers to microns.
- **Grain boundaries:** interfaces where grains of different orientations meet.
- **External surfaces:** interfaces between a solid material and ambient atmosphere.
- **Thermal grooves** form where grain boundaries intersect external surfaces.

**Figure 1:** SEM picture of a network of grains and grain boundaries (Orlandi et.al. 2003). Sintering of a composite material at 1300° C for: (a) 1h; (b) 4h.
Motivation

- **Migration of grain boundary** affects the grain size and orientation, which are influential in defining various properties of metal and ceramic materials.

- Grain boundaries migrate, reducing the **surface free energy** of grains. This motion tends to heal the lattice disorientation and improve the homogeneity of the material.

- **Formation of holes** during grain boundary movement, as well as wetting/dewetting processes, influence the stability of thin metal films which are important in industry.

- Hole formation and dewetting are **undesirable** if the film is designed to protect the underlying substrate, but it can be **useful** in making arrays of nanoscale particles.

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Figure 2: Thermal grooving. AFM from laboratory of E.Rabkin.
A mathematical formulation

Basic modeling assumptions

- Grain boundaries evolve by (isotropic) motion by mean curvature:
  \[ V_n = A H \]
  - \( A \) - reduced mobility, \( V_n \) - normal velocity, \( H \) - mean curvature.

- Exterior surfaces evolve by (isotropic) motion by surface diffusion:
  \[ V_n = -B \Delta_s H \]
  - \( B \) - surface diffusion coefficient, \( \Delta_s \) - the Laplace - Beltrami operator, \( V_n \) - normal velocity, \( H \) - mean curvature.

- Along the contact line, free boundaries, and thermal grooves:
  - Persistence.
  - Balance of mass flux.
  - Balance of mechanical forces: the contact angle \( \theta_c \) is prescribed along the contact curve; the dihedral angle \( \theta_d \) is prescribed along the thermal groove.
Figure 3: Normal cross-section of a thermal groove. \( \theta_d = \pi - 2 \arcsin\left(\frac{m}{2}\right), \quad m = \frac{\gamma_{gb}}{\gamma_s}, \quad x = x(z, t), \quad h = h(x, t). \)

Figure 4: A sketch of contact angles, \( \theta_c \), formed by solid films on substrates. \( \theta_c := \arccos\left(\frac{\gamma_{gs} - \gamma_{fs}}{\gamma_s}\right), \quad h = h(x, t). \)

\[
\frac{x_t}{(1 + x_z^2)^{1/2}} = \mathcal{A} H^{gb}, \\
\frac{h_t}{(1 + h_x^2)^{1/2}} = -\frac{\mathcal{B}}{(1 + h_x^2)^{1/2}} \left[ H^{\text{exterior}}_x \right]_x, \\
H^{gb} := \frac{x_{zz}}{(1 + x_z^2)^{3/2}}, \\
H^{\text{exterior}} := \frac{h_{xx}}{(1 + h_x^2)^{3/2}}.
\]
Experimental motivation: hole growth

Figure 5: AFM images (E.Rabkin).

Figure 6: SEM images of a thin molybdenum (metal) film on a sapphire (ceramic) substrate before after annealing (E.Rabkin).
Experimental motivation: branched shapes

Figure 7: Sample morphologies of dewetting polycrystalline films (SEM images). Thompson, 2012.
Examples of dewetting films with an initially circular hole, $\theta_c = 120^\circ$.

**Figure 8:** A single crystal system.

**Figure 9:** A bi-crystalline system, $m = 0.3$. 

$$a_s = b_s = 1, a_l = b_l = 41, \theta_c = 120^\circ, dt = 1, t = 10$$
Examples of a hole formation and convergence to steady state, $m = 0.3$

**Figure 10:** Hole formation

**Figure 11:** Convergence to steady state.


Thank you for your interest!