COARSENING IN THE NETWORK FLOW

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Solids have a crystalline structure, and a piece of metal is actually (much) more complicated than a unique crystal. Most of the technological materials are polycrystalline: they are composed of several pieces (grains) in which the crystal lattice is rotated in different ways, delimited by grain boundaries. Grain boundaries have a profound impact on materials properties (for instance electrical and thermal conductivity) and therefore their performance. The challenge in polycrystals is then the development of process technology, in other words the way we make materials, that will allow us to arrange grains in a way that gives us the property we desire, these properties can be said strength, toughness, electrical resistivity.

One way that the grain structure is tailored or engineered is through grain growth. To model grain growth is an old problem and it attracted the attention of applied scientists and then mathematicians. Already in 1956, Mullins considered the 2-dimensional version in thin films and observed that the grain boundaries of a recrystallized metal, when annealed, move with a velocity proportional to the curvature [Mul56]. Thus, in a first approximation, the grain boundary and the grain growth can be described as a finite union of curves that meet at junctions (a network) that moves by curvature (the normal velocity of each curvature at each point and time is its curvature). The system evolves so as to reduce the energy, hence we consider the L^2-gradient flow of the length functional and we expect to see networks with only triple junctions at almost all times. The equilibrium state should actually be a single crystal and one of the defining features of evolution is that the network undergoes changes in topology.

It is fair to say that in the last years there have been progresses concerning both in situ–experiments, simulations and mathematical models [Bar+17; ELM21b; ELM21a; KMT]. Unfortunately at the moment experiments cannot give us precise information about the dynamics of the motion of grain boundaries, thus we still have to relies on good models and simulations.

The first attempt to study the network flow from a mathematical point of view has been by Brakke [Bra78], who developed a geometric-measure-theoretic method to define the evolution. While his definition is very powerful and useful in its own way (it provide global existence), it does not give a very detailed picture of the evolution itself, hence the need of a definition based on classical PDE solutions. My final goal is the study of evolution by curvature of cluster of surfaces as a simplified model of grain growth. Concerning the 2-dimensional version, I aim to a complete analysis of the network flow in a PDE framework, from well–posedness, to the study of long–time behaviour and asymptotic analysis as time goes to infinity [Man+16; PT24].

A precise analysis of singularities in some special cases can be used as a benchmark on the reliability of simulations. On the other hand, simulations can be an inspiration for the theoretical study of the flow.

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In numerical simulations we see that the networks completely rearrange itself any time we have a topological discontinuity and larger grains "eat" smaller ones. The most prominent features that eyes pick up is the increasing average size of (surviving) grains [Bra; Ese].

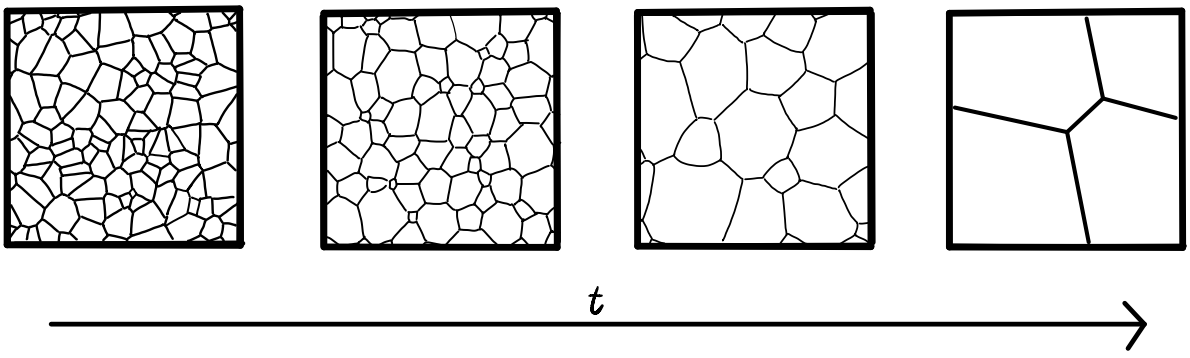

FIGURE 1. Expected evolution of a complicated network

Between the period of critical events we know exactly how the area of a grain grows with time: the grains follow the so-called Von Neumann rule. Consider indeed a grain bounded by a loop ℓ composed of m curves. By Gauss–Bonnet we have

$$\partial_t A = \int_\ell k \, \mathrm{ds} = \left(\frac{m}{3} - 2\right) \pi \,,$$

hence the area of grains bounded by more than six curves grows linearly, by less than six curves decreases linearly and the area of hexagonal cells remains constant. Moreover, by Hölder inequality

$$\left|2 - \frac{m}{3}\right| \pi \leq \int_\ell |k| \leq \left(\int_\ell \kappa^2\right)^{\frac{1}{2}} \sqrt{\mathrm{L}(\ell)} \,,$$

that is

$$\int_\ell \kappa^2 \, \mathrm{d}s \geq \frac{C}{\mathrm{L}(\ell)} \,,$$

with C that is different from zero for non–hexagonal cells. If we suppose that all grains are very similar to each other and the percentage of non–hexagonal grains is sufficiently high during evolution, we can actually formally prove that the average area of the (surviving) grains grows linearly. Consider an initial network composed of N^2 grains in the flat torus and let it evolve by the network flow. We pass from the above estimate on a single grain to the estimate on the entire network simply by multiplying by the number of grains and keeping in mind that the average length of a single loop is of order $1/N$:

$$\int_{\mathcal{N}} k^2 \, \mathrm{d}s \gtrsim N \sharp \left(\text{non–hexagonal grains}\right) = N^3 \,.$$

The evolution law of the the total length of the network reads

$$\frac{d}{dt} L(\mathcal{N}) = - \int_{\mathcal{N}} k^2 \, \mathrm{d}s \,.$$

Now we use the fact that the length of the network is of order N and we put together the last two formula, getting the differential inequality:

$$\frac{d}{dt} N(t) \lesssim -N^3(t) \,,$$

Thus the average area (that is of order $1/N^2$) grows at least linearly in time

$$\frac{1}{N(t)^2} \geq 2Ct\,.$$

It is not difficult to show another property of the flow that indicate that the structure/topology of the networks should be simplified during the evolution. When the flow develops a multiple junction where at most five curves, then the multiple junction will be split in triple junctions and locally all the flowouts will be without loops. Hence, by an easy computation involving the Euler characteristic, one shows that the total number of curves decreases at least by three and the total number of triple junctions decreases at least by two.

To conclude, in my talk I also showed a quantitative estimate of the size of the basin of local minimality of regular networks with straight segments. The estimate, obtained by local calibrations [PP23], indicates that the volume of the basin of attraction of all the many critical points of the length functional is expected to be small in the space of networks hence it is unlikely that the flow gets stuck in a configuration composed of lots of hexagonal grains.

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