Diffusion-limited interface collisions

Bastien Marguet[1], Fabio Reis[2] & Olivier Pierre-Louis[1]

[1]Institut Lumière Matière, UMR5306 Université Lyon 1-CNRS, Université de Lyon, F-69622 Villeurbanne, France

[2]Instituto de Física, Universidade Federal Fluminense, Avenida Litorânea s/n, 24210-340 Niterói RJ, Brazil

Introduction

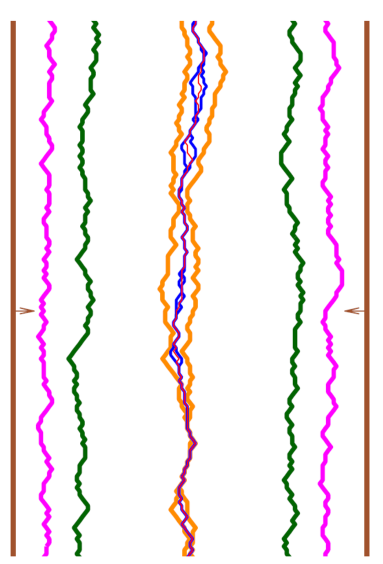
In many growth processes, two-dimensional domains are nucleated, grow, and finally merge. This scenario can be found in diverse non-equilibrium processes [2-5].

We study in details the collision of two straight interfaces moving towards each other and colliding. We focus on the case where interactions are induced by diffusing species, such as during the growth of two-dimensional materials (such as graphene), or during the growth of bacterial colonies competing for food.

We use on-lattice Kinetic Monte Carlo Simulations and find that a linear Langevin model can reproduce the main results.

As opposed to the intuitive expectations, we find that the roughness of the newly formed interface can be smaller when growth is faster. These results could help to minimize the roughness of grain boundaries of grown 2D materials, which have a strong influence on the thermal and electronic transport properties of these materials.

[1]



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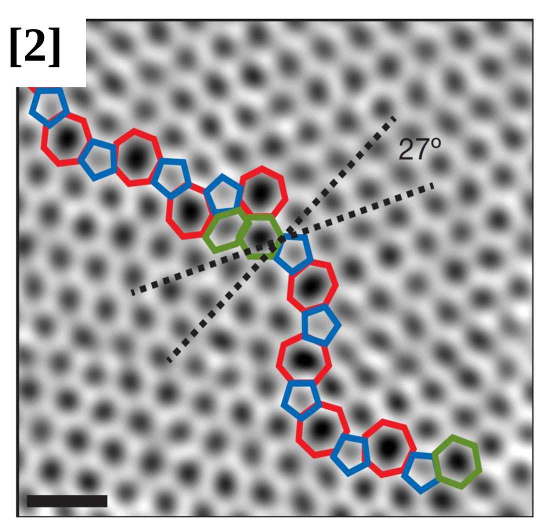
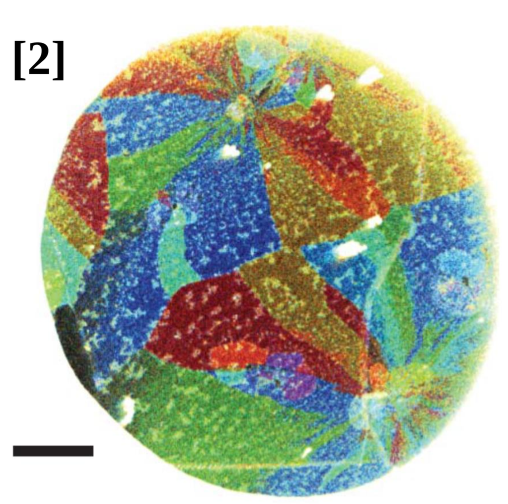


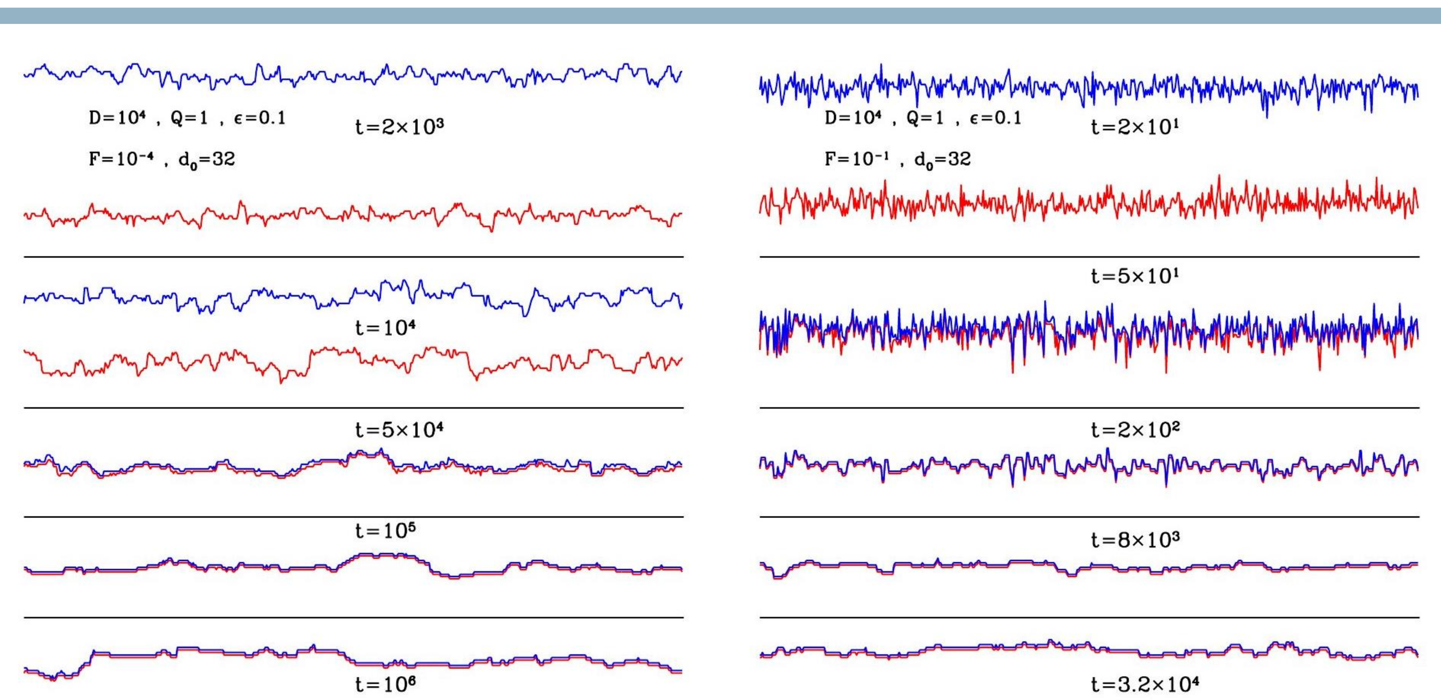
Scale bar is 0.5 nm

[2]



Scale bar is 500 nm

Slow growth vs Fast growth



Dynamics of the spectral roughness

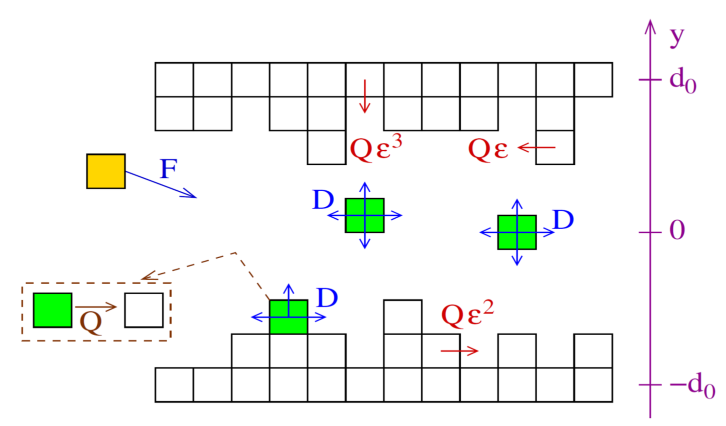
$$\underbrace{\partial_t \left\langle \left|\Sigma h_q^{(1)}(t)\right|^2 \right\rangle}_{\text{Time evolution of the spectral roughness}} = \left(\underbrace{B_{\Sigma q} L}_{\text{Equilibrium noise term}} + \underbrace{2\Omega^2 F h^{(0)} L}_{\text{Out-of-equilibrium noise term}} \right) + \underbrace{2\lambda_{\Sigma q}(t) \left\langle \left|\Sigma h_q^{(1)}(t)\right|^2 \right\rangle}_{\text{Relaxation of the spectral roughness}}$$

Roughness squared

$$\langle\, W^2(t)\, \rangle = \frac{1}{L^2} \sum_{q \neq 0} \left\langle \left|\Sigma h_q^{(1)}(t)\right|^2 \right\rangle$$

Models

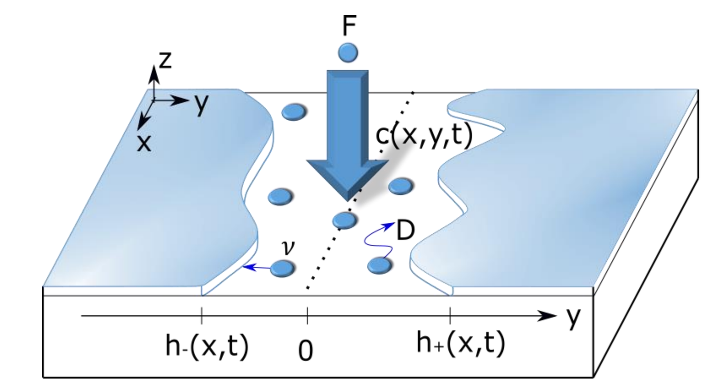
Kinetic Monte-Carlo simulations



2 growing edges of size L:

- Height h±(x,t)
- Flux of growth units F
- Hoping frequency D
- Attachment/detachment kinetic coefficient Q
- No bond between the 2 edges
- Energy bond J ($\varepsilon = e^{-J/k_B T}$)
- Unit area $\Omega = a^2$

Linear Langevin model

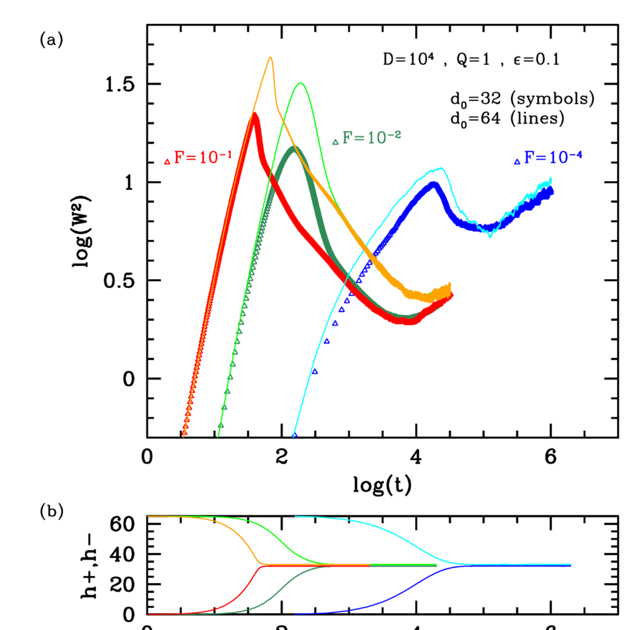


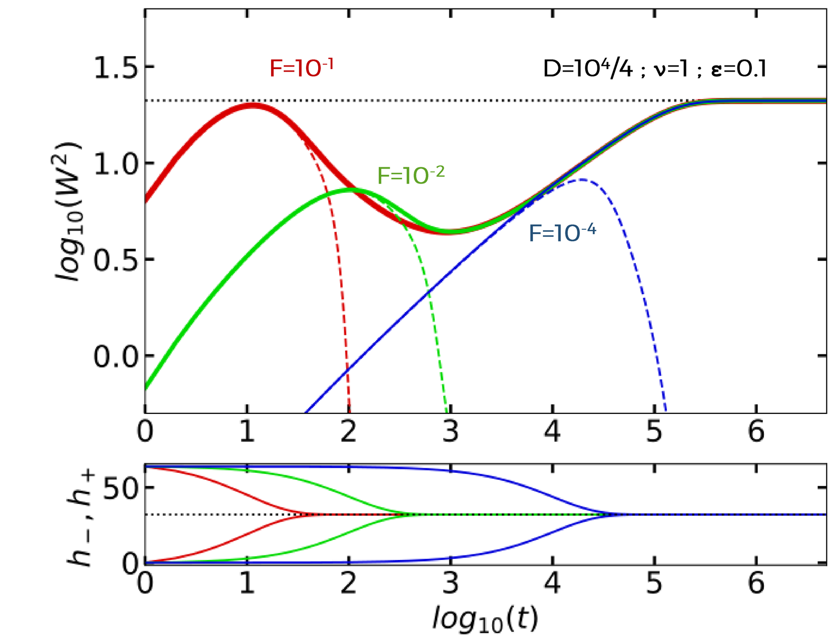
2 growing edges of size L:

- Height h±(x,t)
- Flux of growth units F
- Diffusion coefficient D
- Attachment/detachment kinetic coefficient ν
- No bond between the 2 edges
- Thermal (equilibrium) fluctuations
- Out-of-equilibrium fluctuations

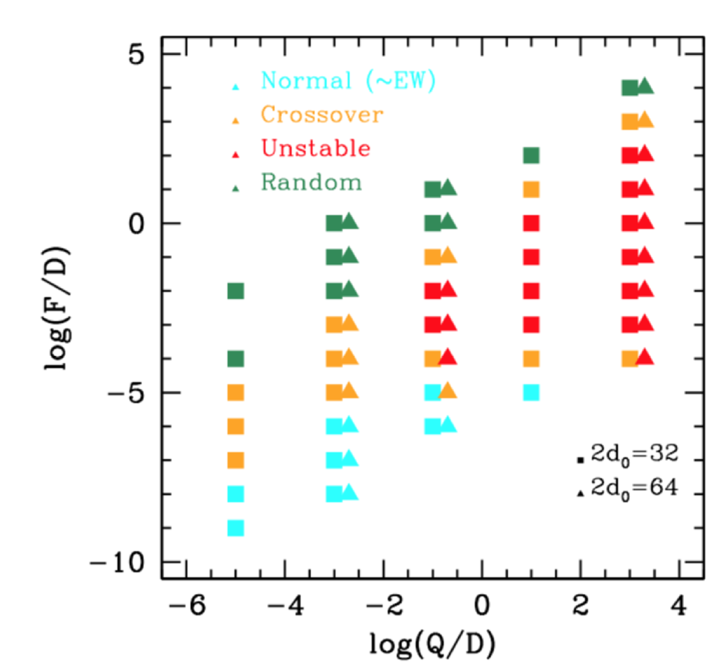
Roughness

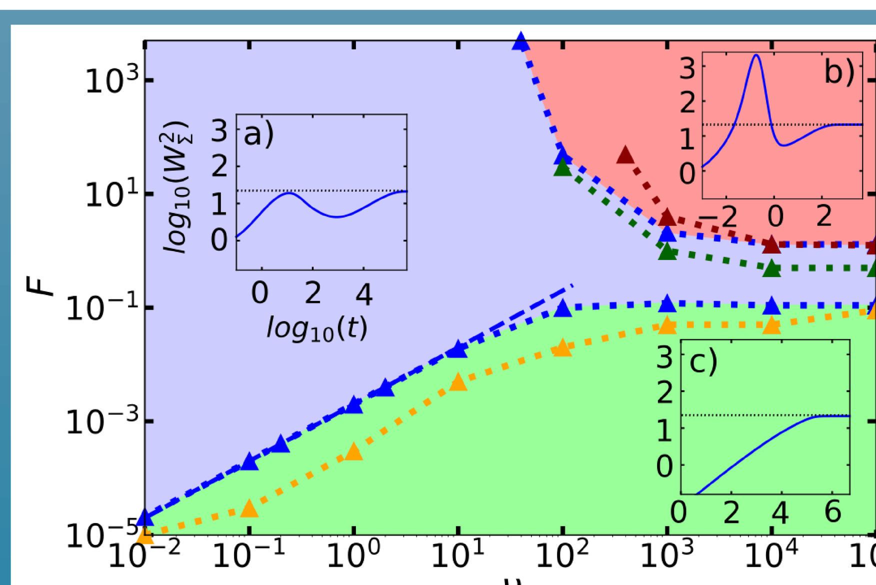
$$W^2(t) = \langle \Sigma h^2 \rangle - \langle \Sigma h \rangle^2$$





Phase diagram





- Green phase: No peak
- Blue phase: Noise dominated peak
- Red phase: Morphological instabilities

Conclusion

Non-monotonous evolution of the roughness in time:

- Peak of roughness before collision + Drop after collision ($W_\Sigma \approx a$) + Relaxation
- A faster growth can lead to a smaller roughness
- Linear Langevin model in agreement with Kinetic Monte-Carlo model

Phase diagram:

- 3 different regimes:

→ Low flux (slow growth) and fast kinetics: no peak of roughness
→ High flux (fast growth) and slow kinetics: peak + drop of roughness
→ High flux and fast kinetics: morphological instabilities

Perspectives:

- Comparison with experiments

References

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Contact person

Bastien Marguet

bastien.marguet@univ-lyon1.fr

Acknowledgments

Université Claude Bernard Lyon 1

iLM Institut Lumière Matière

CNRS

Universidade Federal Fluminense