GRAPHENE AND 2DM VIRTUAL CONFERENCE & EXPO

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GRAIN BOUNDARY FORMATION IN TWO-DIMENSIONAL MATERIALS

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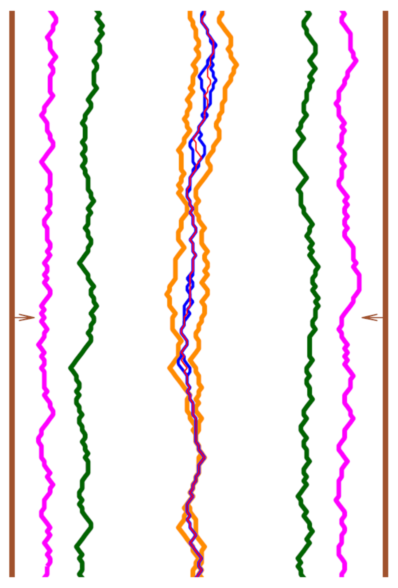
Introduction

[1]



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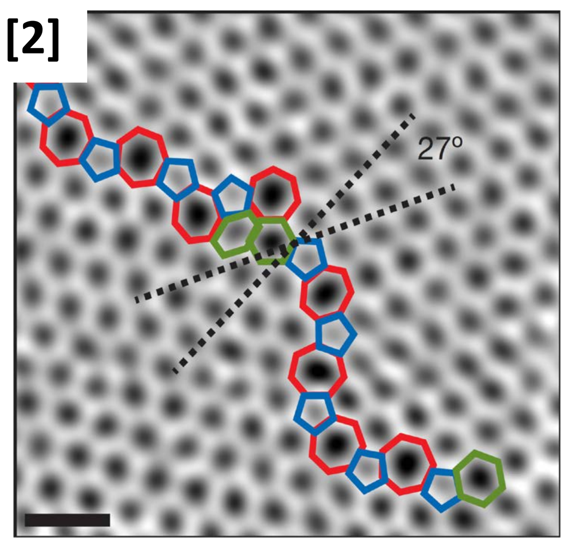

Scale bar is 0.5 nm

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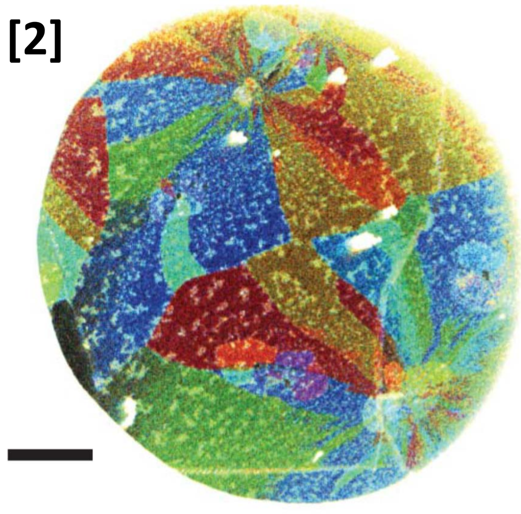


Scale bar is 500 nm

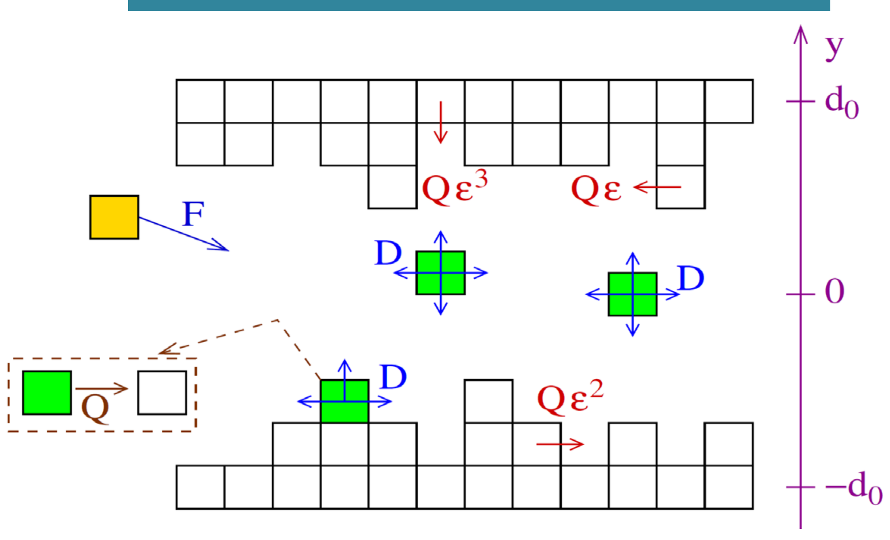
The roughness of grain boundaries in 2D materials strongly influences physical properties such as mechanical strength, electronic and thermal conductivities. However, the process by which rough grain boundaries are formed during growth is still poorly understood.

Our model aims at describing the formation of rough grain boundaries in epitaxially grown 2D materials such as graphene. Grain boundaries are formed by the collision of two rough growing edges. We provide a detailed description of the statistical fluctuations and morphological instabilities of the edges during the growth process using both Kinetic Monte-Carlo Simulations and an analytical Langevin model.

Our models predict the existence of a sharp decrease of the edge roughness during the collision of two edges. This decrease is enhanced during fast growth, leading to the counter-intuitive conclusion that fast growth could give rise to flatter/smoother grain boundaries.

Models

Kinetic Monte-Carlo simulations



2 growing edges of size **L**:

- Height **$h_\pm$(x,t)**
- Flux of growth units **F**
- Diffusion coefficient **D**
- Attachment/detachment kinetic coefficient **Q**
- No bond between the 2 edges

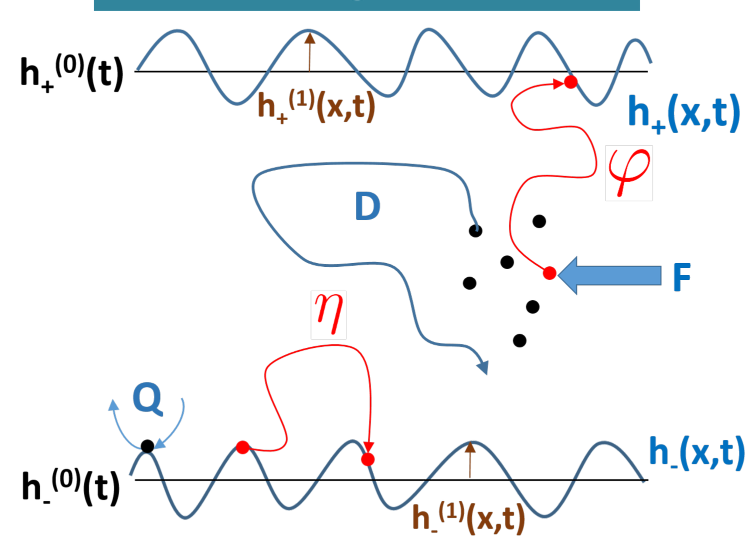
Kinetic Monte-Carlo model

- Energy bond **J** ($\varepsilon = e^{-J/k_B T}$)
- Unit area **Ω** = a^2

Langevin model

- Thermal (equilibrium) fluctuations **η**
- Out-of-equilibrium fluctuations **ϕ**

Linear Langevin model



Results

Linear Langevin equations

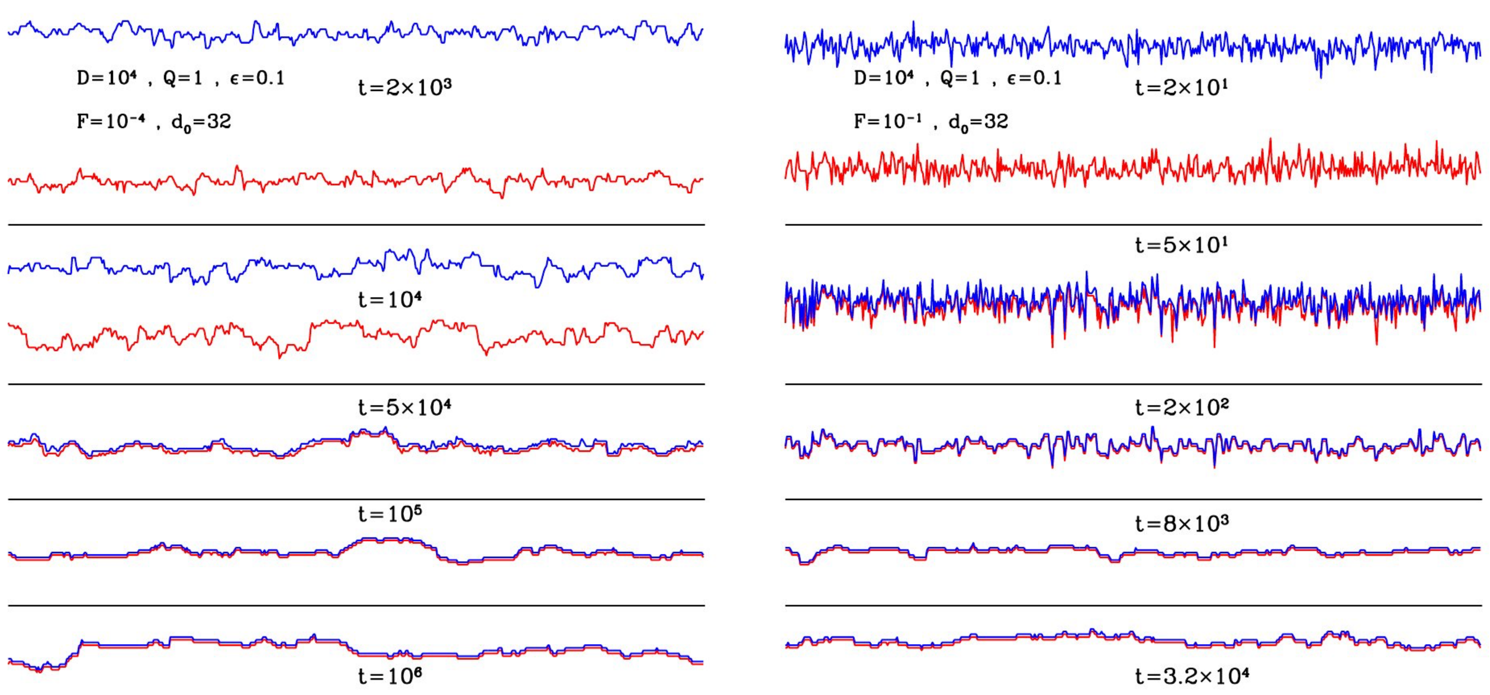
Dynamics of the spectral roughness

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

Roughness squared

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

Slow growth VS Fast growth

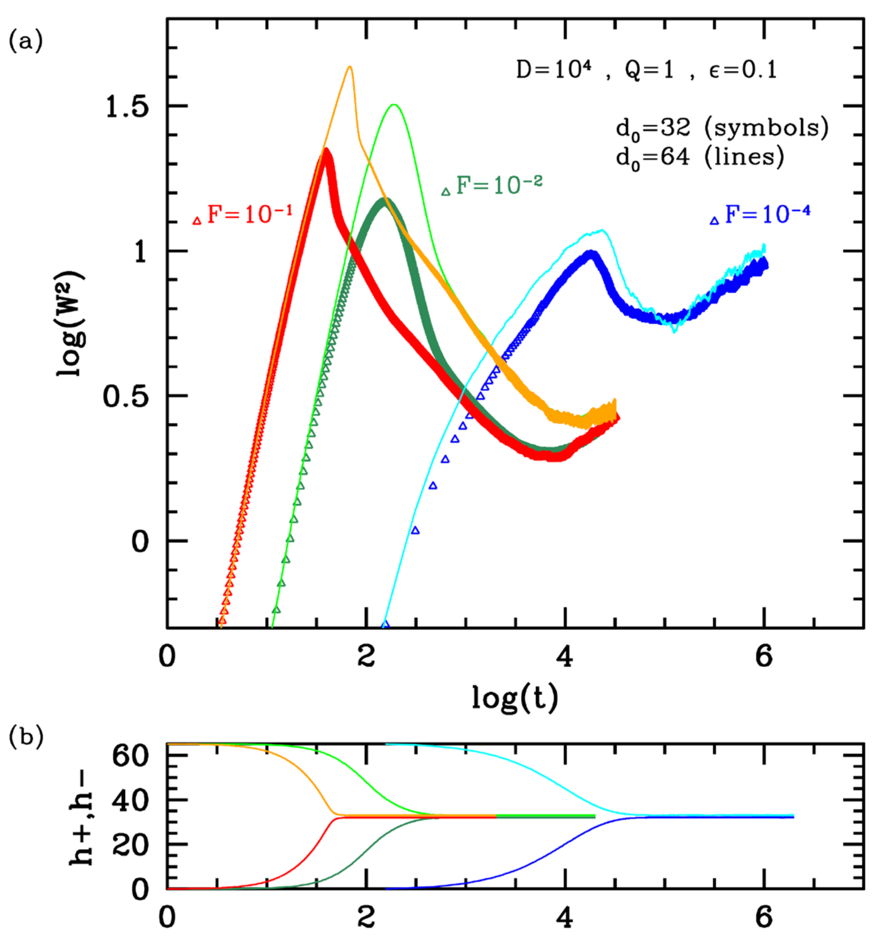


Slow growth | Fast growth

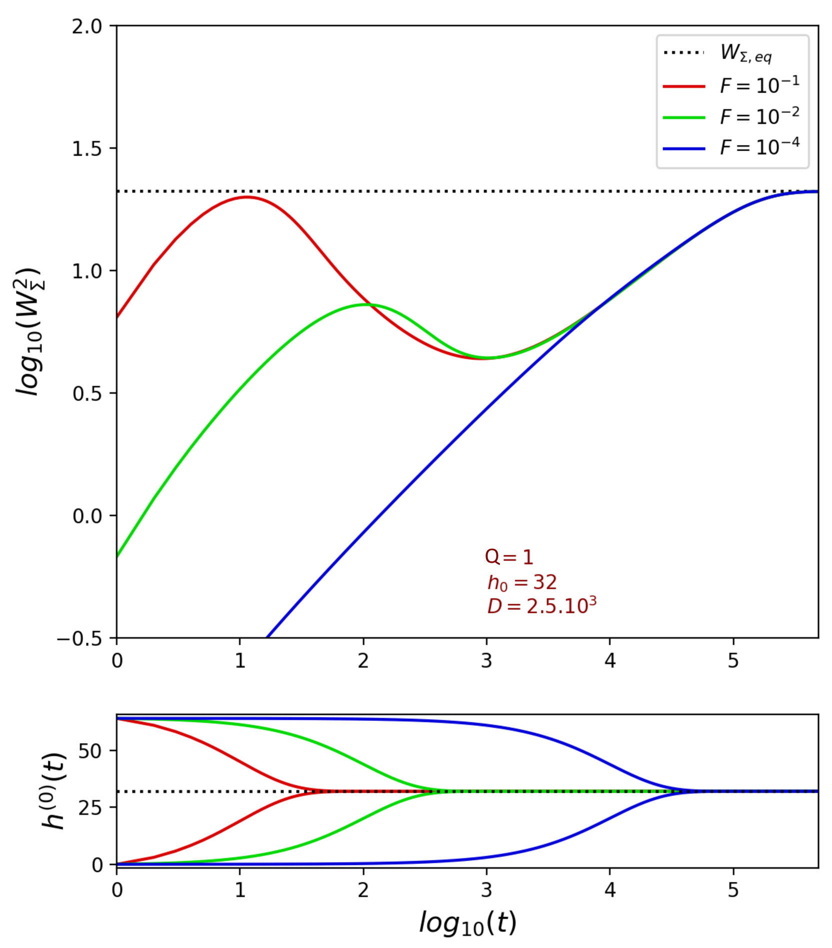
Evolution of the roughness

Roughness: variance of the interface height

$$W = \sqrt{W^2} = \sqrt{\frac{1}{L}\int_0^L dx\,(h(x,t))^2 - \left(\frac{1}{L}\int_0^L dx\, h(x,t)\right)^2}$$

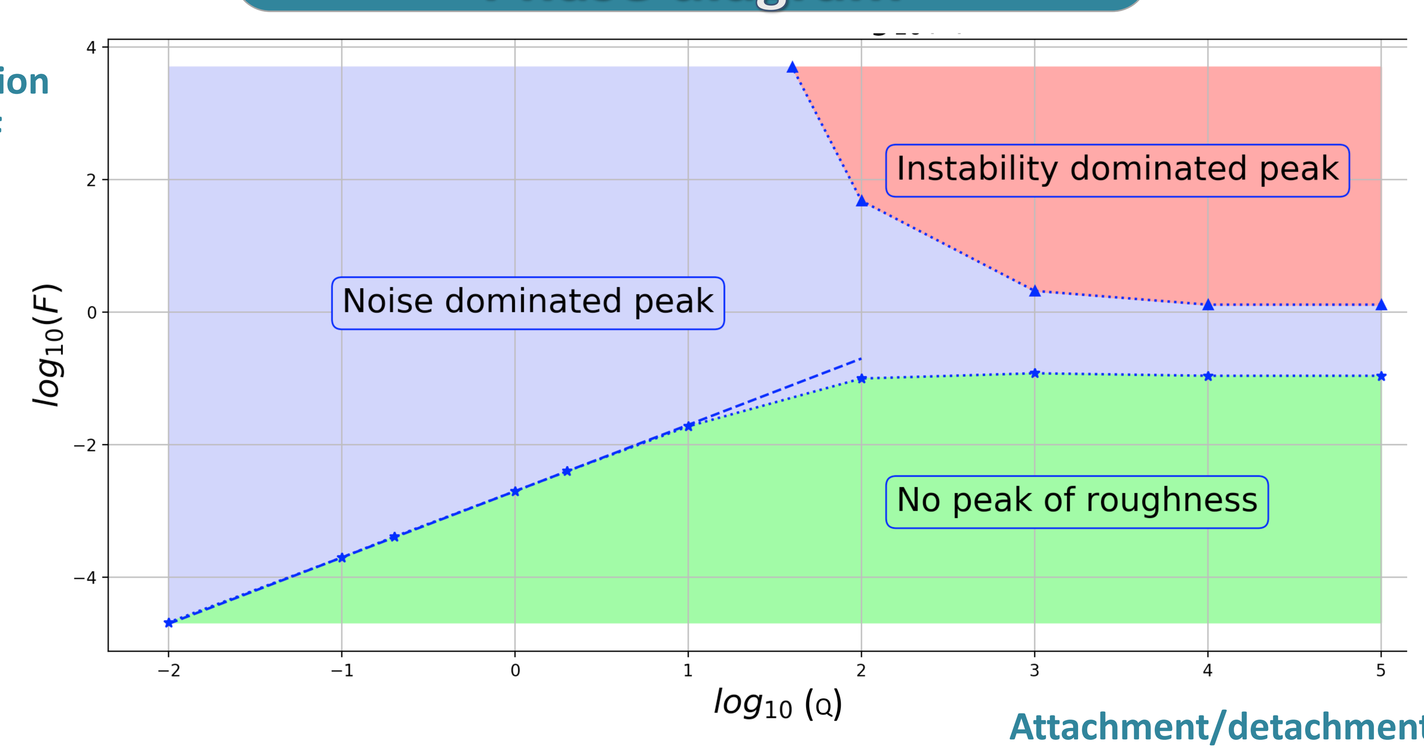


Kinetic Monte-Carlo simulations



Linear Langevin model

Phase diagram



Deposition flux F

Attachment/detachment kinetics Q

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

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REFERENCES

[1] F. D. A. Aarão Reis and O. Pierre-Louis, Physical Review E 97, 040801(R) (2018)

[2] P. Y. Huang & al., Nature (London) 469, 389 (2011)

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