II Miniworkshop

Statistical Mechanics applied to growing materials under nonequilibrium conditions

This workshop, the second in a series that began in 2022, focuses on Statistical Mechanics modeling of growing materials under nonequilibrium conditions. This research field significantly contributes to nanoscience and nanotechnology, as well as other areas where complex surface phenomena need to be addressed. One of its advantages is representing surface processes in a simplified yet consistent manner with reality, facilitating the interpretation of models and results. Moreover, the models describe the materials production processes rather than analyzing the physical properties of already formed structures. Consequently, the results can be useful for predicting more suitable material production conditions.

Date: Thursday (02/05/2024)

Time: 2pm (Seminar room - 412 – 4th floor of IF-UFBA)

Program

(14:00) **Simulating growth of nanostructured materials to relate their microscopic dynamics with their morphologies**, Fábio David Alves Aarão Reis (IF-UFF) [Pg. 3]

(14:40) **Restoring the fluctuation-dissipation theorem in phase transition through a new emergent fractal dimension**, Fernando Albuquerque de Oliveira (IF-UnB/IF-UFF) [Pg. 4]

- Cofee Break (15:20 – 15:40)

(15:40) **Accessibility of the surface fractal dimension during film growth**, Edwin Edgar Mozo Luis (IF-UFF) [Pg. 5]

(16:20) **Effects of the probe diameter of an electrostatic force microscope on the topography measurements of rough interfaces: a computational simulation approach**, Thiago Albuquerque de Assis (IF-UFBA/IF-UFF) [Pg. 6]

(17:00) **Scaling corrections in nonequilibrium (d+1) surface growth**, Pablo Menezes Amorim (IF-UFBA) [Pg. 7]

(17:40) **Machine Learning-Based Prediction of Temperature-Like Parameters in Nonlinear MBE Growth Models**, Bassem Y. J. Makhoul (Polytechnic School - Electrical Engineering Program - UFBA) [Pg. 8]

Simulating growth of nanostructured materials to relate their microscopic dynamics with their morphologies

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This talk summarizes recent works to describe the morphology of growing materials using simulations of kinetic models properly designed for different deposition techniques. First, we study island growth, coalescence, and initial formation of continuous heteroepitaxial films with a vapor deposition model [1]. A framework is proposed to relate the evolution of the surface roughness and of height correlations with step-edge energy barriers and atom/molecule diffusivities on the substrates. When those barriers are negligible, the roughness shows a maximum as the islands coalesce, as observed in hot-wall CdTe deposition on polyimide substrates and in thermally evaporated perovskite films. Next, using models of electrodeposition with adsorbate diffusion, we show initial compact film formation followed by instability development and dendrite growth [2]. The application to silver electrodeposition on nanoparticulated gold substrates explains the transition from microparticles with (111) facets to pine-tree shaped dendrites which preferentially grow from the corners and edges of those particles [3]. The adatom diffusion coefficients in the electrodeposited structures can be obtained from their characteristic sizes and the applied currents. An application to Fe films electrodeposited on Si(100) helps to explain the secondary nucleation of Fe grains during the crossover from compact to dendritic growth [4]. Finally, using a model of sputter deposition, we obtained morphologies similar to those of hybrid Si films with Ti nanoparticle scaffolds, which were developed for anodes of Li ion batteries. The talk will also summarize our recent studies of the universal features of roughness scaling in film deposition models with Ehrlich-Schöwebel (ES) barriers at step edges [5].

[1] T.B.T. To, R. Almeida, S.O. Ferreira, F.D.A.A. Reis, Appl. Surf. Sci. **560**, 149946 (2021).
[2] D. di Caprio, A. Taleb, F.D.A.A. Reis, J. Phys. Chem. C **122**, 21418 (2018).
[3] S. Dokhan, D. di Caprio, A. Taleb, F.D.A.A. Reis, ACS Appl. Mater. Interfaces **14**, 49362 (2022).
[4] L. Benetti et al, Cryst. Growth Des. **23**, 7958 (2023).
[5] I. S. S. Carrasco, T. B. T. To, F. D. A. A. Reis, Phys. Rev. E **108**, 064802 (2023).

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Restoring the fluctuation-dissipation theorem in phase transition through a new emergent fractal dimension

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We develop the hypothesis that the dynamics of a given system may lead to a fractal dimension d_f different from the original spatial dimension d. This phenomenon is more easy to observe near a phase transition. We also speculate how the response function might be sensitive to this change in dimensionality. We discuss how this phenomenon appears in phase transition and growth phenomena. Furthermore, we show that correlations appear as the difference between $d - d_f$ becomes sensitive, an effect similar to what occurs in growth phenomena [1-6]. Moreover, we determine [7] the Fisher exponent as $\eta = d - d_f$, and the fractal dimension d_f for the Ising model. We validate it via computer simulations for two dimensions [7].

[1] M. S. Gomes-Filho and F. A. Oliveira, EPL **133**, 10001 (2021).
[2] P. R. H. dos Anjos, W. S. Alves, M. S. Gomes-Filho, D. L. Azevedo and F. A. Oliveira, Frontiers in Physics **9**, 741590 (2021).
[3] M. S. Gomes-Filho, A. L. A. Penna and F. A. Oliveira, Results in Physics **26**, 104435 (2021).
[4] E. E. M. Luis, T. A. de Assis, F. A. Oliveira, Journal of Statistical Mechanics: Theory and Experiment, 083202 (2022).
[5] E. E. Mozo Luis, F. A. Oliveira, and T. A. de Assis, Phys. Rev. E **107**, 034802 (2023).
[6] M. S. Gomes-Filho, Pablo de Castro, D. B. Liarte, and F. A. Oliveira, Entropy **26**, 260 (2024). https://www.mdpi.com/1099-4300/26/3/260
[7] H. A. Lima, E. E. M. Luis, I. S. S. Carrasco, A. Hansen, F. A. Oliveira. arXiv preprint arXiv:2402.10167.

Accessibility of the surface fractal dimension during film growth

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Fractal properties on self-affine surfaces of films growing under nonequilibrium conditions are important in understanding the corresponding universality class. However, measurement of the surface fractal dimension has been intensively investigated and is still very problematic. In this investigation, we report the behavior of the effective fractal dimension in the context of film growth involving lattice models believed to belong to the Kardar-Parisi-Zhang (KPZ) [1] and Villain Lai Das Sarma (VLDS) [2,3] universality classes. Our results, which are presented for growth in a d-dimensional substrate (d = 1, 2) and use the three-point sinuosity (TPS) method [4], show universal scaling of the measure M, which is defined in terms of discretization of the Laplacian operator applied to the height of the film surface. We show the scale limits within which the TPS method can be used to determine the effective fractal dimension, where the results are consistent with the KPZ class. We compared these results with those obtained using the height difference correlation [5] function and the Higuchi method [6]. Furthermore, we extend these discussions to a model in which the dominant ingredient is diffusion during film growth and find that the TPS method only extracts the corresponding fractal dimension in the steady state [7].

[1] M. Kardar, G. Parisi, and Y.-C. Zhang, Phys. Rev. Lett. **56**, 889 (1986).
[2] J. Villain, J. Phys. I (France) **1**, 19 (1991).
[3] Z.-W. Lai and S. Das Sarma, Phys. Rev. Lett. **66**, 2348 (1991).
[4] Y. Zhou, Y. Li, H. Zhu, X. Zuo, and J. Yang, Fractals **23**, 1550016 (2015).
[5] D. O. Mallio and F. Aarão Reis, Physica A **596**, 127178 (2022).
[6] T. Higuchi, Physica D **31**, 277 (1988).
[7] E. E. M. Luis, F. A. Oliveira, and T. A. de Assis, Phys. Rev. E **107**, 034802 (2023).

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Effects of the probe diameter of an electrostatic force microscope on the topography measurements of rough interfaces: a computational simulation approach

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In this talk, I will explore, through computational simulation, how the tip diameter (ε) of an electrostatic force microscope (EFM) operating at a constant force influences the determination of the growth exponent (β) during film deposition on a one-dimensional substrate. Laplace's equation is solved within the EFM simulation framework using the finite element method to compute the electrostatic force between the tip and the film interface. It's worth noting that for EFM tips with sufficiently large apex diameters, the topographies obtained from EFM closely resemble those derived from the transformed mean height profile (TMHP) method. In this approach, the interface is partitioned into bins of equivalent tip diameter, and the average height within each bin is utilized to transform the original interface. This correspondence is established within lattice models representing the Kardar–Parisi–Zhang (KPZ) and Villain–Lai–Das–Sarma (VLDS) classes. I will discuss a scale relation between global roughness and tip diameter, setting a threshold value for ε where a reliable KPZ/VLDS growth exponent can be determined using EFM under constant force. Notably, if the diameter of the EFM tip exceeds the surface correlation length, a spurious effective growth exponent consistent with uncorrelated growth is observed [1].

[1] P. M. Amorim, E. E. M. Luis, F. F. Dall'Agnol and T. A. de Assis, J. Appl. Phys. **133**, 235304 (2023).

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Scaling corrections in nonequilibrium (d+1) surface growth

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We investigate the existence of scale corrections in lattice models in higher dimensions and propose a new measure that can mitigate scale corrections. Confirming recent results of Mallio and Reis [1], we show that also for $d \geq 2$, on a scale of the order of the lattice parameter the height difference correlation function $G_d(s)$ scales with $s^{2\alpha}$, with the same exponent expected in the hydrodynamic regime. However, we emphasize the existence of an additional term $\phi(a/s)$ that modifies the scaling relationship and is responsible for corrections on scales of the order of the lattice parameter. Furthermore, we introduce a family of statistical measures, $\psi_k(s)$, based on the linear combination of height difference correlation functions at different scale lengths. Our analytical analysis showed that this function is more effective in reducing scale corrections at small wavelengths when compared to other quantities already reported in the literature, such as the TPS method and the height difference correlation function. Additionally, we study the scale corrections associated with intrinsic roughness that modify the Family-Vicsek ansatz, implementing corrections to the global quadratic roughness. The study carried out by Alves *et al.* [2], indicates that intrinsic roughness is associated with stochastic height fluctuations in narrow and deep valley regions. In this sense, we use the optimization method known as Lagrange multipliers and show that the profile that minimizes the intrinsic roughness is equal to the transformed mean height profile (TMHP), introduced by Amorim *et al.* [3]. Using the TMHP method in lattice models belonging to the KPZ class, in 1+1 dimensions, such as the Ballistic deposition model and the Etching model, we note that it promotes scale corrections in the local roughness and provides a greater scale range and plateau for obtaining the effective exponent of local roughness, α_{loc}.

[1] D. O. Mallio and F.D.A.A. Reis, Physica A **596**, 127178 (2022).

[2] S. G. Alves, T. J. Oliveira, and S. C. Ferreira, Phys. Rev. E **90**, 052405 (2014).

[3] P. M. Amorim, E. E. M. Luis, F. F. Dall'Agnol and T. A. de Assis, J. Appl. Phys. **133**, 235304 (2023).

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Machine Learning-Based Prediction of Temperature-Like Parameters in Nonlinear MBE Growth Models

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The Clarke–Vvedensky (CV) model represents a noteworthy contribution in the field of stochastic modeling applied to molecular-beam epitaxy (MBE). This technique has considerable attention due to its effectiveness in producing high-quality thin films. Notably, MBE films have various applications, including the production of devices like transistors and light-emitting diodes. The CV model, in its original form, is characterized by temperature-like parameters, namely: the diffusion-to-deposition ratio of isolated atoms on terraces (R) and the detachment probability at step edges (ε). This work systematically investigates various combinations of R and ε values through kinetic Monte Carlo simulations in a low-temperature regime, generating data on surface topographies at different deposition times. Subsequently, machine learning models, specifically ensemble models, are utilized for a precise classification and identification of R and ε values for surfaces not encountered during the training stage. Remarkably, our data preprocessing methodology achieves an accuracy rate of approximately 98% in predicting R and ε for a surface topography based on just one independent realization in our simulation. Further research towards more realistic models incorporating the Ehrlich-Schwoebel barrier mechanism is desirable and is in progress. We hope that our technique can be useful to interpret images depicting surface topographies of films precisely measured with probe microscopies, aiming to assist in the development of microscopic models that describe the key mechanisms contributing to the production of technologically relevant films.

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