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Aug 8, 2023, České Budějovice

Opponent's report of a doctoral thesis

Kinetic Monte Carlo Simulations in Physics of Thin Films: from Growth to Electronic Properties
by
Mgr. Vít Gabriel
submitted at the **Faculty of Mathematics and Physics, Charles University**
in the field
Physics of Plasmas and Ionized Media

The thesis is focused on computer simulations applying kinetic Monte Carlo to studies of plasma deposition processes and thin film growth. The work is nicely linked to experiments that provide benchmark data that are used to tune the simulation parameters and provide data for comparison and testing of various models. This comparison allows to infer the role of various processes of layer-by-layer deposition.

The results of the student's work are summarized in the thesis' conclusion. I particularly like the novel model for the simulations of PLD growth avoiding simulations of diffusion of individual adatoms, assuming instantaneous equilibration leading to a homogeneous distribution of adatoms within a layer. This method and its implementation are clearly explained in Chapter 2. I also like the discussion of the results. This Chapter is based on three papers with the student as a first author and his excellent orientation in this research is evident.

Chapter 3 is based on a preprint where the student was a third author but in addition it includes figures and details not present in the archived manuscript. I like the introduction to this part, but the description of the work is less clear, and particularly the discussion of results, description of a search for the best parameters, etc. are brief, leaving a number of points unclear.

I appreciate that even though the student published three first-author publications and co-authored another manuscript, the thesis is written in a stand-alone form, which enhances the readability of the thesis. The thesis is well-written (with only a few typos and error in noun-verb correspondence) and easy to follow, the results and algorithms are well-documented.

Summary: The student convincingly demonstrated that he is able to pursue scientific ideas motivated by real processes and experiments, implement them efficiently in computer simulations, obtain and discuss in depth the results and draw conclusions shedding new light on the modeled processes.

I therefore fully support awarding him the Ph.D. degree.

Below I list a few deficiencies I found in the thesis and I would be happy to discuss at least some of my questions and comments during the defense.

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Critical points:

1) The very first introductory paragraph on page 4 is hugely oversimplified and even incorrect.
2) A "≤" condition must appear once in step 5, page 5.
3) Fig. 2.1 lacks a legend or explanation in the caption of the different curves.
4) Upper summation bound $h>h_{max}$ in eq. (2.8) is incorrect.

Questions to the student and suggestions for a discussion:

Q1: Guess what I strongly dislike in the first introductory paragraph on page 4, correct and discuss this paragraph.

Q2: In section 2.1 (page 8), an experimental deposition frequency 0.02 Hz is cited, but section 2.2 (page 10) describes that "To reproduce the PLD growth experiment, it was necessary to simulate at least a square with an edge length of one micrometer for approximately two hours of deposition with 5 Hz laser frequency". Please explain this difference in frequencies. Are they normalized per surface area?

Q3: In Fig. 2.4, arbitrary units of SXRD axes are mentioned, but the text on page 12 and the definition of SXRD, eq. (2.2) indicate that the scale is not arbitrary, but ⟨0,1⟩.

Q4: Fig. 2.8b shows slopes with exponents β = 0.3, 0.5, and 0.7. Is there any special reason to choose these values?

Q5: On page 21 you write "We assume that there is no physical reason why the energy barriers E_i should depend on *f*. If the opposite were true, it would mean that the most fundamental processes on the surface are dependent on some external events". Can you imagine a situation when this assumption would not be valid?

Q6: 'Correlation length' is presented in Fig. 2.13, though in the preceding paragraph it is referred to as the 'average island diameter'. I assume both terms refer to identical property. Please explain its definition, since the statement "The average island size is calculated by autocorrelation of the given surface and determination of the correlation length." lacks details (autocorrelation of which property?). Note that 'correlation length' is mentioned in the thesis before only on page 8, but in a different context (of the X-ray).

Q7: Do you have any explanation for the two linear regions in Fig. 2.13b?

Q8: From Fig. 3.1 it is evident that the polaronic diffusion is experimentally measured via the 'outside potential' between the surface and AFM tip. However, the simulations were carried out in a 3D cubic lattice. Is it plausible to link these two setups and their results? In Figure 3.7 a geometry resembling a narrow parallel slab is presented, which further confuses me about the choice of studied geometries.

Q9: In Chapter 3, two processes are considered – i) injection of a polaron and ii) jumps of polarons. As a result, their number just grows. Should not some decay of polarons be introduced?

Q10: Are the data presented in Chapter 3 going to be published in another form than the arXiv preprint?

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