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Simulating the formation of fuzz on the wall of a fusion reactor

-*Introduction*:

Given the pressing concerns inherent to energy production from fossil fuel, it is of utmost importance to develop novels means of producing safe, clean and cheap energy. One of the possible solutions to this problem is nuclear fusion (NF). In NF, light nuclei are fused together to produce heavier elements, which typically also releases very energetic neutrons. The energy of these neutrons can then be harvested in order to produce electricity.

One of the main issues facing NF energy production is that materials that can withstand the extremely hostile conditions necessary for fusion are not currently available. The present project addresses one of these challenges: the formation of so-called nanoscale “fuzz” at the surface of the first-wall material of fusion reactors. The formation of this fuzz can compromise the mechanical integrity of the material or promote the formation of dust, which can pollute the plasma. The main objective is to develop a simple, yet representative, model to understand the mains processes that lead to fuzz formation. Eventually, that could help researchers to mitigate the deleterious effects of surface modifications.

-*Technical background*:

Currently, the leading design for energy production calls for the fusion of deuterium and tritium to form helium, a neutron, and 17.6 MeV of energy (most of it carried away by the neutron). Given the extremely high temperature required to induce fusion (tens of millions of degrees K), the resulting plasma cannot be mechanically contained; instead it is contained by an electromagnetic field. Despite of this containment, a considerable flux of high-energy neutrons will hit the wall (this is in fact essential to extract energy from the reactor), as well as some hydrogen isotopes and helium (the fusion product). In the case of the so-called divertor (currently made of tungsten), helium and hydrogen impact the surface with only about 50 eV of energy, an amount that is only sufficient to penetrate a few nm inside the wall.

Despite this relatively soft landing, it is now understood that this intake of He can cause dramatic surface morphology changes, most notably the growth of bubbles or fuzz (a dense forest of small tendrils that grow out of the surface). To try to understand this effect alone, without any of the other complications of the full fusion environment, careful He plasma experiments have been performed. In these experiments, the temperature is controlled and the surface is bombarded by He ions at a specific energy, typically a few tens of eV. Some results are illustrated in Fig. 1.

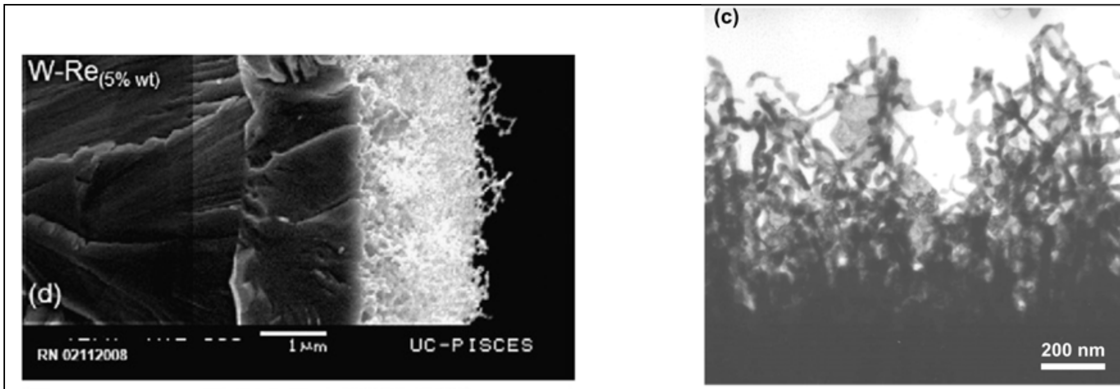

Figure 1: Formation of fuzz on tungsten surfaces exposed to an He-containing plasma. Left: exposure at 1120K, He energy=40eV [1]; right: exposure at 1400K, He energy=50eV [2].

We believe that the process of fuzz formation can be captured by a relatively simple kinetic model. We suggest an on-lattice kinetic Monte Carlo approach, where the atomic-scale evolution of the surface is simulated from the knowledge of the basic unit processes that can occur. The main challenge of the project is to define, parameterize and implement a kinetic model that embodies these essential elements. The model should be as simple as possible, but not more!

We believe that the essential features are as follows:

- Tungsten (W) and He atoms sit on either substitutional (between W atoms) or interstitial sites
- W and He can diffuse to neighboring sites
- He atoms coming from the plasma are implanted into the W surface
- He atoms bind to other He atoms
- W atoms bind to other W atoms
- He atoms are repulsed by W atoms
- Sufficiently large interstitial clusters of He (~8) will eject an W atom (creating a W interstitial) creating an immobile bubble
- Bubbles can grow by ejecting W atoms to create new W interstitials
- Bubbles that grow to the point of touching the surface burst, getting rid of their He.

-***Special Requirements****:*

none

- ***Expectations****:*

The main goal of the project is to develop a kinetic model that can be used to understand the nature of the process that leads to the formation of fuzz and to identify the main parameters that control fuzz formation. The idea is not to carefully choose the value for every single parameter, but to identify the generic features that a model should have to form fuzz, in a setting that is consistent with the basic physics of the problem. It would also be very interesting to understand the impact of the different parameters on the fuzz formation efficiency, i.e., identify the key parameters that control how fast fuzz can grow.

If appropriate, and if time permits, the development of simple analytical or semi-analytical models that helps in understanding the results would be very desirable.

-***Recommended Reading****:*

Introduction to Kinetic Monte Carlo:

Arthur F. Voter, Introduction to the kinetic Monte Carlo method, in Radiation Effects in Solids, Springer, pp. 1-23 (2007)

Tungsten fuzz:

[1] M.J. Baldwin and M. Doerner, Formation of helium induced nanostructure 'fuzz' on various tungsten grades, Journal of Nuclear Materials 404, 165–173 (2010)

[2] Shin Kajita *et al.*, TEM observation of the growth process of helium nanobubbles on tungsten: Nanostructure formation mechanism, Journal of Nuclear Materials 418, 152–158 (2011)

A. Lasa *et al.*, MD simulations of onset of tungsten fuzz formation under helium irradiation, Nuclear Instruments and Methods in Physics Research B 303, 156-161 (2013)