Multiscale modeling of ion beam interactions with materials from the quantum to the mesoscale

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The theoretical treatment of ion beam interactions with materials has relied heavily on atom-level computer simulations since the 1950's, when the binary collision approximation and molecular dynamics simulations were developed. Since then, the applicability of the methods has developed heavily due to advances in both computer capacity and methodology. While the first simulations were carried out with very approximate classical pair potentials, it is nowadays possible to simulate low-energy irradiation effects with fully quantum mechanical models, and the classical potentials have evolved into being able to take into account complex chemical bond conjugation effects.

In this talk, I will present a brief overview of the main atom-level methods currently used to simulate radiation effects and diffusion of the implanted atoms, namely quantum mechanical and classical molecular dynamics and kinetic Monte Carlo.

I will then present recent examples of their use, including determining the threshold displacement energy surface in silicon quantum mechanically [1], the role of bond conjugation chemistry in fusion reactors [2], as well as how impurity migration, trapping and bubble growth can explain the recently observed effect of 'fuzz' formation in W [3].

References

[1] E. Holmström, A. Kuronen, and K. Nordlund, Phys. Rev. B 78, 045202 (2008)
[2] A. Meinander, C. Björkas, and K. Nordlund, The effect of hydrocarbon chemistry on sputtering in mixed Be-C-H materials, Nucl. Instr. Meth. Phys. Res. B 303, 188 (2013).
[3] A. Lasa, K. O. E. Henriksson, and K. Nordlund, Nucl. Instr. Meth. Phys. Res. B 303, 156 (2013).