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Kinetic Monte-Carlo modeling of plasma-surface interactions with realistic surfaces

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Despite the remarkable progress in ab-initio modelling of plasma-surface interactions, atomistic simulations on time and length scales that are relevant to real experimental systems remain challenging. Therefore, coarse-grained deterministic models are often used in plasma modeling. In deterministic description, surface kinetics is formulated in terms of fractional coverages of different types of active sites and simulated by a system of differential equations. Such mesoscopic approach is simple and computationally efficient but it is inherently approximate because it does not account for the complex microscopic details of the underlying processes. In this presentation, Kinetic Monte Carlo(KMC) modelling of surface kinetics in reactive plasmas is discussed. We demonstrate that KMC is particularly well suited to bridge the gap between the complexity of atomistic simulations and the effectiveness of deterministic models. In KMC approach, the master equation for a given system is not explicitly solved, but instead the underlying Markov process is simulated numerically. KMC algorithms are exact, they can handle reaction probabilities that depend on the local configuration of the system and they are well suited to model heterogeneous surfaces that exhibit distributions of adsorption energy and reactivity. In this report, KMC modelling of atomic recombination and molecular formation on surfaces in contact with reactive plasmas is discussed. Simulations are benchmarked against the available experimental data. In particular, surface processes in systems with a distribution of active sites is analyzed in detail.