KINETIC MONTE CARLO ALGORITHMS FOR SURFACE KINETICS

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In this report we present and discuss the interest and efficiency of Kinetic Monte Carlo (KMC) algorithms to study heterogeneous atomic recombination and molecule formation [1]. KMC simulations are then used to validate deterministic calculations, where surface kinetics is formulated in terms of fractional coverages of different types of adsorption sites, described by a system of reaction-rate differential equations. The cases of NO oxidation on Pyrex and O recombination on silica forming O2 and O3 are discussed in detail.

Acknowledgments: VG was partially supported by FCT, Projects UID/FIS/50010/2013 and PTDC/FIS-PLA/1420/2014 (PREMiERE)

1. V. Guerra and D. Marinov, *Plasma Sources Sci. Technol.* **25** (2016) 045001.
2. D. Marinov, C. Teixeira, V. Guerra, **Plasma Process. Polym. 14** (2017) 1600175.