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Molecular dynamics study of the formation of porous films by room-temperature physical vapor deposition of silica

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Low-temperature physical vapor deposition is studied by means of molecular dynamics (MD) simulations using the reactive force field (ReaxFF) potential. In contrast with prior MD studies of this process, which employed non-reactive, rigid ion force fields, our approach allows for accurate modeling of the reactive incorporation of impinging particles, generated by the vaporization process, into the growing film. The use of the ReaxFF force field also enables us to properly model the charges of impinging particles and their electrostatic interactions with the atoms forming the topmost layers of the growing film. In order to better evidence the associated effects, we focus on the conditions of growth when the impinging particles have moderate kinetic energies (below a couple of electron-volts). We thus evidence that, in these conditions, impacting particles tend to be strongly deflected during the last stages of their approach to the film, and all the more so that they are slow. As a result, they tend to be captured by denser regions, leading to the formation of porous microstructures. This phenomenon results from the polarization of \ce{Si-O} bonds, and the tendency of silicon atoms to surround themselves with oxygen atoms, leading to an overall polarization of the interface between dense matter and pores.

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