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PROC / Process control (including plasma diagnostics, plasma modelling)

Reaction of neutral species in homogeneous phase in molecular dynamics simulation of Ar/CH_4 plasma

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Abstract content

Molecular dynamics is used to mix the majority neutral species constituting an Ar/CH_4 plasma in the homogeneous phase. The composition of this plasma and the molar fraction of each species is obtained from a 1D model. The mixing is done at temperatures of 300k, 400k, 500k and 1000.

Complex Non-Equilibrium Hydro-Carbon Plasmas are weakly ionized gases containing electrons, neutral and charged molecular species, large clusters and possibly solid particles. They are today a major tool for the elaboration of carbon materials and advanced nanostructures and several key applications in the field of microelectronics.

It is often difficult to study surface and homogeneous phase reactions experimentally because industrial processes are often established on the basis of empirical challenges and not on the basis of a thorough understanding of the physico-chemical mechanisms involved. Molecular dynamics simulations are natural methods for analyzing these phenomena because they provide insight into the mechanisms between species.

The mixing of these neutral species by molecular dynamics simulation has allowed to study the interaction between these molecules and the reaction in the homogeneous phase. This allowed to observe a conservation of the molecules C_2H_2, C_2H and the disappearance of CH_4 whatever the temperature. The formation of other species has also been observed.

MDs are carried on by mixing a total number of 519 molecules that takes into account the molar fraction, with a time step of 0.25fs. The simulation box is calculated according to the reference [1].

C-C and C-H interactions are described with the REBO potential whereas Ar-C and Ar-H interactions are modelled using Lennard-Jones potentials.

Thanks/Acknowledgement

This work was partly supported by the French National Research Agency (ANR) through the MONA project (ANR-18-CE30-0016)

References

[1] P. Brault, « Multiscale Molecular Dynamics Simulation of Plasma Processing: Application to Plasma Sputtering », Front. Phys., vol. 6, p. 59, juin 2018, doi: 10.3389/fphy.2018.00059.