Dynamics of Biphenylene Carbon (Graphenylene) Hydrogenation.

Vinicius Spluges (IC), Pedro A. S. Autreto (PQ), Douglas S. Galvão (PQ).

Abstract

We report here a fully reactive molecular dynamics study on the structural and dynamical aspects of the hydrogenation processes of Biphenylene Carbon (BPC) membranes. BPC is porous graphene-like two-dimensional allotrope carbon. Our results show that BPC hydrogenation exhibits very complex patterns but in contrast to graphene, the formation of correlated hydrogenated islands was not observed.

Key words: Nanotechnology, molecular dynamics, graphene.

Introduction

With the advent of graphene, there is a renewed interest in carbon-based structures. Graphene and several of its derivatives present a great number of interesting physical properties, which can be exploited in many applications, such as, membranes. There is a great interest in discovering new graphene-like porous membranes. Biphenylene carbon (BPC), sometimes called graphenylene, is one of these structures. BPC is a porous two-dimensional (planar) allotrope carbon form and presents a very interesting topology, with its pores resembling typical sieve cavities in some zeolites. In this work, we have investigated BPC hydrogenation dynamics under different conditions (hydrogenation plasma density, temperature, etc.).

Results and Discussion

The hydrogen incorporation processes on BPC were studied through molecular dynamics (MD) techniques using reactive force field ReaxFF, as implemented in the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) code.

The systems considered in our simulations are composed of BPC membranes (initially with dimension ~120 Å x 120 Å, about 5000 carbon atoms) embedded into a pure H atmosphere, using a constant volume box (NVT ensemble). We considered different hydrogenation plasma densities, because it is well-known that in some cases extensive hydrogenation can lead to the formation of defective areas and structural holes.

We investigated the dynamics of hydrogenation at different temperatures (300 K, 600 K and 800 K). Our results show that hydrogen incorporation rates are very sensitive to temperature values and extensive hydrogenation produced significant structural damages.

In image 1 we present a representative snapshot from MD simulations of the hydrogenation process at 300 K, where we observed the absorption of hydrogen takes place at the top and bottom of the membrane, but there is not a perfect pattern to follow.

Image 1. Representative snapshot from the MD simulation of the H atoms (represented in yellow) incorporation process.

Conclusions

Our results show that the BPC hydrogenation processes exhibit very complex patterns, but the formation of correlated domains (islands) observed in the case of graphene hydrogenation, do not occur. Also, extensive hydrogenation can produce significant structural damages, with the formation of large defective areas and structural holes. In these aspects BPC hydrogenation exhibits patterns closer to the ones reported to graphene fluorination.

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References