Molecular dynamics simulation of Ion Beam Etching as technology process for creating graphene-based membranes

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Abstract – Carbon nanomaterials present new possibilities for creating permeable membranes. Ionic beam etching technology allows to create pores in graphene substrates and has the potential to be used in various separation processes. In our study we present a molecular dynamics simulation of the energy needed to puncture the graphene surface to create porous surface. Experimental part shows dependency of irradiation time to pore diameter on silica substrate, which indicates it is possible to create pore diameters lesser than the beam diameter. We present a technology process of creating pores of a specific diameter.

Keywors – graphene, membrane, transport, ion beam, molecular dynamics.

Introduction

According to the definition, a membrane is a "structure, having lateral dimensions much greater than its thickness, through which mass transfer may occur under a variety of driving forces" [1]. Membranes processes can separate particles and molecules and over a wide particle size range and molecular weights. Efficiency in a membrane process is determined by a selectivity parameter. Unique structure of a one atom thick sp^2-bonded carbon sheet of graphene presents unique properties than other forms of carbon in context to membranes. It has large theoretical specific surface area and even with pores its structure remains very resistant to pressure. It has potential for being a material to create very selective and permeable membranes, with personalized pore diameter for various processes e.g. gas separation, electrodialisys, nanofiltration [2]. Functionalizing its surface it further changes the properties of a porous membrane created from graphene sheet. As shown in the MIT computational study, transport of water through nano-porous graphene-oxide membranes could reach up to 66 L/cm2/day/MPa with greater than 99% salt rejection. [3]. Creating a porous surface on a graphene can be carried out by focused ionic beam etching and it is possible to influence the pore diameter with respect to irradiation time and the by choosing an optimum angle [4].

In our work we use classical molecular dynamics code with a focus on materials modeling to develop a technology for creating a technological process for creating porous surface on graphene.

Simulation and experiment

We present the process for creating reliable molecular dynamics model of graphene surface ion beam etching carried out for various pore diameters. In our approach the model of single and several graphene sheets are hit by a fullerene model to imitate the energy density of ion beam. We created a dependency graphs of kinetic energy to pore diameter using several different fullerenes models. To our simulation we used the AIREBO [5] force field potential, which is a good system for modeling carbon and/or hydrogen atom interactions. The deflection of fullerene model indicates that with optimal angle and low enough kinetic energy it is possible to create pores of smaller diameter than the ion beam diameter.

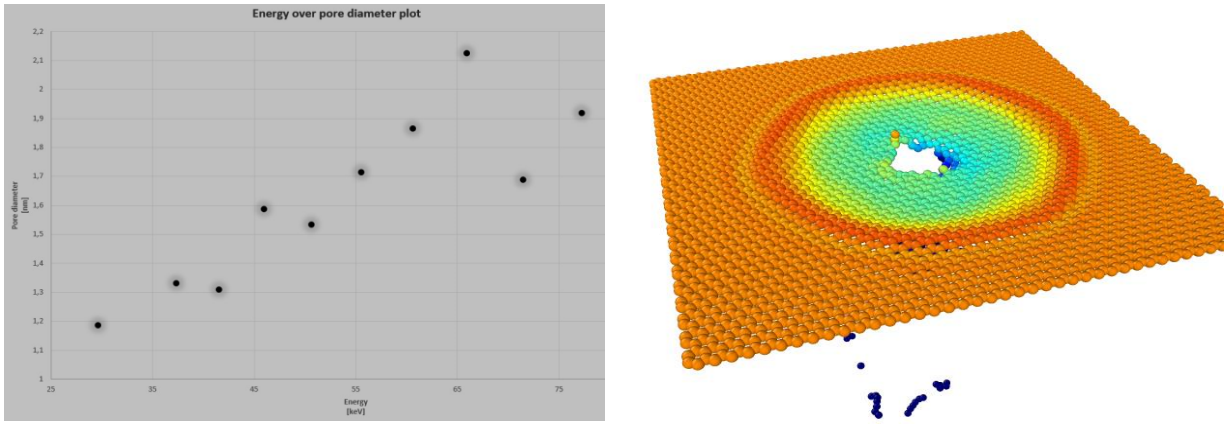

Figure 1. Left: Dependency of energy density to pore diameter in C180 fullerene model simulation, Right: Graphical representation for the impact simulation in molecular dynamics model created by LAMMPS package [6] with Ovito plugin [7]

Experimental part was to create a dependency of the pore diameter to the irradiation time. It was carried out with ionic beam etching on a silicon substrate.

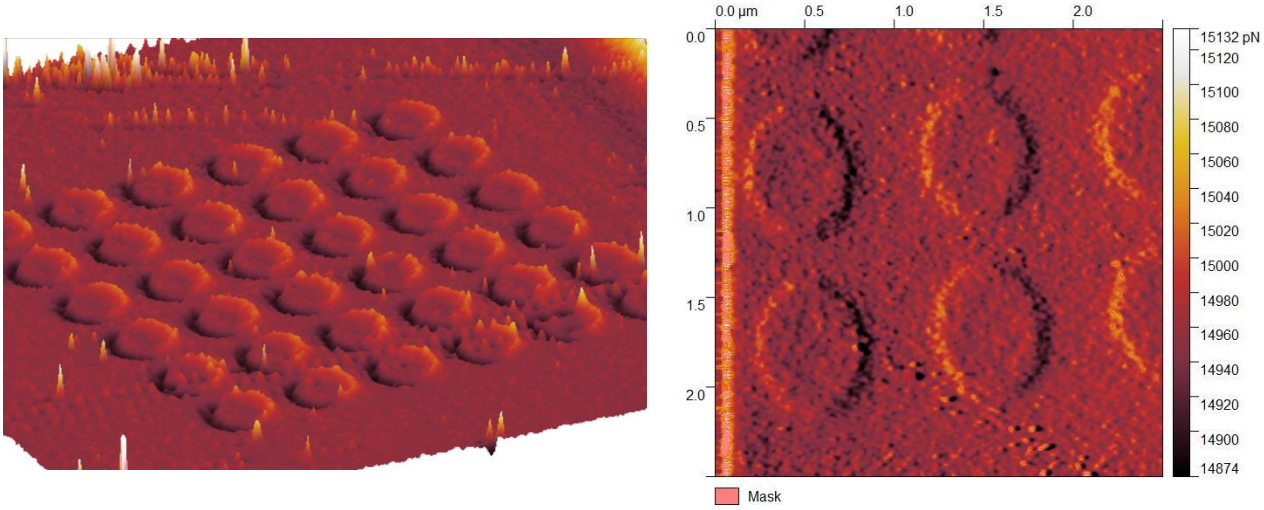

Figure 2. AFM pictures of Silicon substrate after FIB etching done in Nanores company in Wrocław.

Conclusion

The molecular dynamics model can very well be used to imitate the ion beam irradiation on the graphene surface. The characteristics of graphene's response to ion irradiation can be used to gain detailed control over produced defect types. This information is needed in order to controllably create porous membrane from this material, and then to create a experimental installation using this type of molecular sieve.

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