GATES: nanoporous GrAphene membrane made without TransfEr for gas Separation

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Abstract

Up to now, two kind of graphene-based membranes for gas filtration applications have been made: very selective membranes produced by adding graphene oxide on porous materials, or less selective membranes, exhibiting an excellent permeance due to the atomic thickness of graphene decorated with nm size pores. GATES project aims at making the proof of concept at a TRL level 3 of a new membrane based on CVD graphene, offering simultaneously both, high selectivity (103) between H2 (He) and CO2, N2, O2, Ar gases, and a high permeance (10-5 mol m-2 s-1 Pa-1). The project's concept lies on technological innovations for both device's and pores' fabrication, which will offer these outstanding membranes' performances. Concerning device fabrication, we propose a ground-breaking approach overcoming roadblock graphene's technology based on transfer methods for single-layer CVD graphene (SLG). Indeed, SLG approaches based on transfer techniques are very limiting for industrialization processes. Furthermore, they induce high amounts of macroscopic defects, decreasing the yield of membranes' production. GATES developments for devices' fabrication will provide suspended SLG membranes of high quality and permeance, without employing any transfer step. In addition, this proposed procedure will be compatible with a CMOS technology, ensuring manufacturability. Membranes possessing very high selectivity require sub-nanometer pores' diameter. In GATES, nitrogen doping, favoring 3N-pyridinic vacancies on the SLG, will be created by electron cyclotron resonance (ECR) plasma. These vacancies will be further etched if needed. As an alternative approach, we will evaluate nano-pores fabrication by using heavy ions. In both cases, a comprehensive statistical study on pores' shapes, sizes and atomic configurations will be developed by advanced TEM analyses. These statistics will be used as input parameters for the modeling of the membrane performances. In the project, the filtering properties of pristine and N-doped nano-porous graphene will be calculated by different first-principles approaches. This modeling work will support the experimental developments and will be used to identify the optimal structure for the best permeability/selectivity ratio. GATES will also assess the porosity due to grain boundaries, by simulating different local environments, i.e. different pentagons-heptagons configurations.Finally, two SLG devices will be stacked together to increase the selectivity by adding tortuosity. Theoretically, we will also evaluate a further step for improving selectivity, which will consist in the functionalization of these double-layer graphene structures. Eventually all developments, included in GATES project, based on unique graphene membranes, and their application to leak detection, will offer a significant innovative product for users, providing a highly portable/integrated device with a very short response time.

Consortium

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