Atomic-Scale Simulations of High-κ Dielectrics Deposition on Graphene

Bora Karasulu, Wilhelmus M. M. Kessels and Ageeth A. Bol

Eindhoven University of Technology, Department of Applied Physics,
De Zaale, 5612 AZ Eindhoven, The Netherlands
b.karasulu@tue.nl

Abstract

Graphene-based transistors (GFETs) have the potential to enable the transparent, flexible, cost-efficient and high-performance electronic devices of the future.[1] For building GFETs, integration of graphene with ultra-thin layers of high-κ dielectrics (metal oxides) is essential.[2] To this end, atomic layer deposition (ALD) is the method of choice due to its unique control over film thickness, uniformity and chemical content, high film quality and conformality without requiring high operational temperatures.[3,4] However, the deposition of dielectrics on graphene using ALD (or any other technique) poses a genuine challenge due to its chemical inertness. Graphene needs to be activated for surface reactions, but this activation may also degrade its outstanding electronic and mechanical properties.

To tackle this issue, we performed an elaborate modelling study using *ab initio* density functional theory (DFT) with a plane-wave basis, so as to design superior ALD strategies that would enable pinhole-free, closed thin-film formation on graphene without compromising its excellent properties. Strong binding of the precursor on graphene, through either physisorption or chemisorption, is the key for a proper ALD nucleation (see Figure 1). In this respect, this talk will address the binding affinities of a comprehensive list of ALD precursors (e.g. TMA for Al_2O_3, etc.) for pristine graphene and its derivatives with functional groups (e.g. graphene oxide, etc.) or defects (e.g. grain boundaries). Our results show that specific ligand types, especially aromatic ones, facilitate precursor binding; in view of them, we propose novel ALD precursors with improved affinity for pristine graphene. Besides, we will also discuss how a graphene support (e.g. copper, graphite, etc.) affects the binding of ALD precursors. In particular, our results show that Cu(111) -a substrate commonly used for growing graphene- can significantly assist the precursor binding on graphene and its derivatives (see Figure 1).

References

[1] Ferrari, A. C. et al. *Nanoscale* **2014**, *7* (11), 4598–4810.
[2] Morozov, S. V. et al. *Phys. Rev. Lett.* **2008**, *100* (1), 11–14.
[3] George, S. M. *Chem. Rev.* **2010**, *110* (1), 111–131.
[4] Knoops, H. C. M. et al. In *Handbook of Crystal Growth: Thin Films and Epitaxy*; Thomas F. Kuech, Ed.; Elsevier B.V.: Oxford, U.K., **2014**; Vol. 3, pp 1101–1134.

Figures

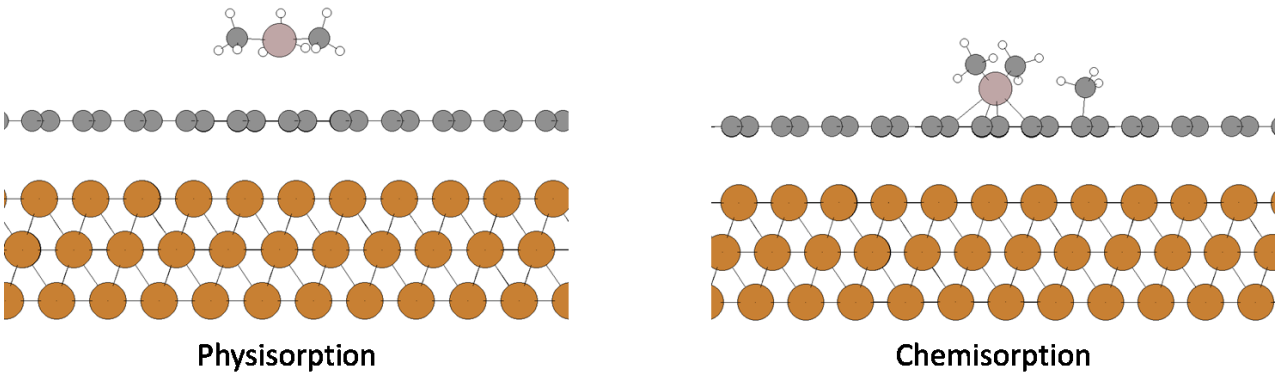

Figure 1. Adsorption of a trimethylaliminum (TMA) precursor for Al_2O_3 ALD on graphene placed on a Cu(111) substrate.