Defects Production at Epitaxial Graphene on SiC using Multi-scale Modelling Techniques

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Abstract

In this study, we present a detailed analysis of single, double and complex vacancies formed in epitaxial graphene on SiC using density functional theory and molecular dynamics simulations. The effect of substrate is explicitly considered in forming defects. The information about the number, types and location of defects produced in each layer of EG is required for producing engineered defects for their various applications [1]. The choice of ions and the energy ranges are such that the production of defects can be controlled. The He FIB (operating at 30 keV) have been previously used to produce defects in EG on SiC [2]. Hence, we have considered the ion energy ranges within the operating range of Helium Ion Microscope (HIM).

References

[1] C. P. Huelmo, M. G. Menezes, R. B. Capaz, and P. A. Denis, Phys. Chem. Chem. Phys. 22, 16096 (2020)

[2] M. Heilmann, V. Deinhart, A. Tahraoui, K. Höflich, and J. M. J. Lopes, npj 2D Materials and Applications 5, 70 (2021).

Figures

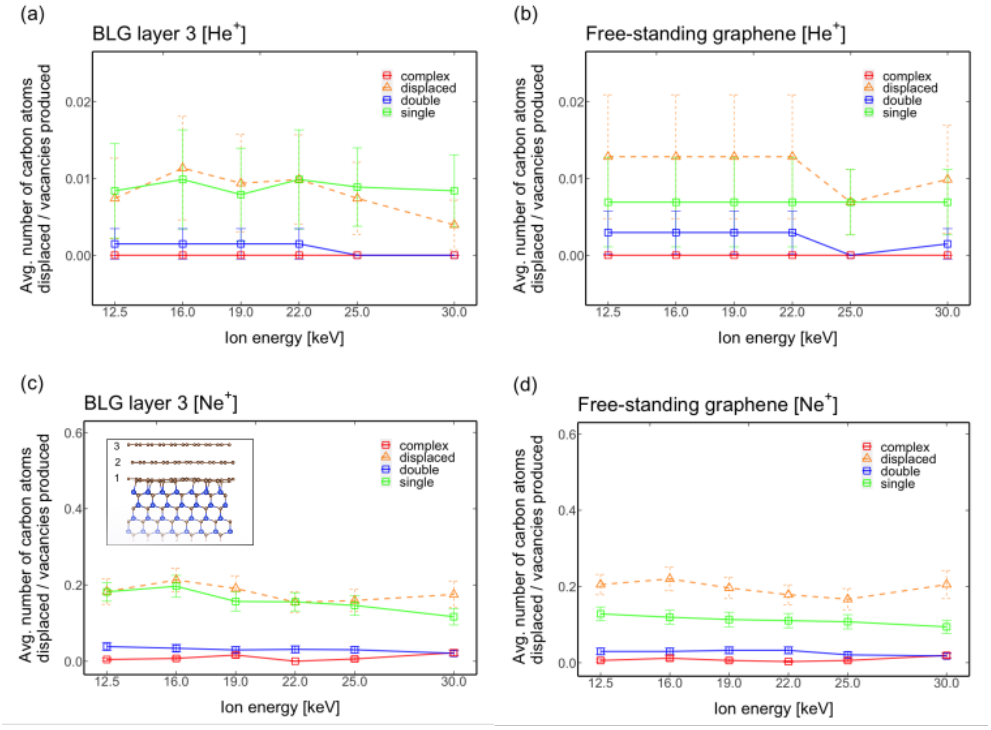

Figure 1: The average number of different types of vacancies (single, double and complex) produced from single He/Ne ion impact on (a, c) BLG top layer and (b, d) free-standing graphene.