

Abstract Submitted
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Epitaxial growth mechanisms of graphene and effects of substrates¹ V. ONGUN OZCELIK, SEYMUR CAHANGIROV, SALIM CIRACI, Bilkent University — Graphene growth and energy barrier calculations of defect healing were investigated using ab-initio MD calculations[1]. It was found that there are two mechanisms which play crucial roles in the growth of graphene. First mechanism is the formation of large carbon rings at the edges which eventually collapse to form honeycomb structure with defects. This collapse is found to be initiated by the new coming carbon atoms which replace one of the bonds in the ring, and expands it until the critical size is reached. Second mechanism is the formation of PH defects near the edge and their healing. We have shown that the energy barrier needed to overcome during healing of the PH defects are much lower than that of the SW defects. We have shown that the presence of a BN or Ni substrate have crucial effect on growth. These substrates guide the formation of honeycomb structures from carbon rings and enable the healing of specific defects as growth proceeds. We also studied graphene growth using carbon dimers as building blocks and found that defect formation is less frequent as compared to growth with monomers.

[1] V. Ongun Ozcelik, S. Cahangirov and S. Ciraci, Phys. Rev. B 85, 235456 (2012)

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V. Ongun Ozcelik
Bilkent University

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