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Dislocation and pentagon-heptagon pair generation in vacancyinduced graphene layer BYOUNG WOOK JEONG, HOONKYUNG LEE, Department of Physics and Astronomy, Seoul National University, GUN-DO LEE, Department of Materials Science and Engineering, Seoul National University, JISOON IHM, Department of Physics and Astronomy, Seoul National University — We investigate the mechanism of the generation of long range order defects in graphene layer by tight binding molecular dynamics simulations and first-principles total energy methods. It is found that the vacancies are diffused and coalesced to make the dislocation defect with the two 5-7 pair defects when more than a certain number of vacancies are present. We examine the magic number of the vacancy which gives dislocation defects in a graphene layer. STM simulation results related to the graphite lattice with the period of $\sqrt{3} \times \sqrt{3}$ in an STM topograph will be discussed.

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