Mutual transformations between divacancy defects induced by high-energy pulses in graphene

***Jun Xia, †HengAn Wu**

Department of Modern Mechanics, University of Science and Technology of China, China

*Presenting author: xiajun@mail.ustc.edu.cn
†Corresponding author: wuha@ustc.edu.cn

Abstract

The introduction of defects and their structural evolutions in graphene are essential in tailoring the exceptional properties and thereby performances of graphene-based devices, such as nanoporous membranes for the filtration and desalination of water. To clarify the underlying mechanism in defect evolutions, we investigate the mutual transformations among the four typical divacancy defects in graphene induced by a high-energy pulse, using molecular dynamics simulation. Six possible mutual reaction paths are revealed in the transformation process, during which defects transform by absorbing energy to overcome the energy barrier with bonding, debonding, and bond rotations. The reversibility of defect transformations is studied by potential energy analysis. If the energy difference between the reactant and product defects is too large, the potential direct transformation path will be irreversible or even impossible. Moreover, the correlation between the transformation probability and the input energy indicates the existence of a local maxima at an optimal input energy, which should provide an optimized strategy to dramatically increase the transformation probability between defects by using high-energy pulses.

Keywords: Graphene, Defect, Transformation, Reversibility