

Abstract Submitted
for the DFD14 Meeting of
The American Physical Society

Enhancement of Sublimation of Single Graphene Layer by Interacting with Gas Molecules in Rarefied Environment¹ RAMKI MURUGESAN, JAE HYUN PARK, Gyeongsang National University — Graphene has excellent mechanical properties. One of them is the resistance to high temperature environment. Since the sublimation temperature of graphene is over 4500 K, it has been used for diverse high temperature applications in order to protect the system. In this study, using extensive molecular dynamics simulations, we show that the sublimation of graphene could be enhanced (occurs at the lower temperature) by interacting with the gas molecules. With increase in temperature, the bonds in graphene become so sensitive to interact with the incoming gas molecules. When the temperature is low, the graphene is stable to the impingement of gas molecules: The light H₂ gases stick to the graphene surface and remain being attached while the heavy CO₂ and H₂O are bounced back from the surface. However, at high temperature H₂ gases are absorbed on the graphene and destroy the C–C bonds by forming C–H bonds. The local breakage of bond at the impingement spot spreads the entire graphene soon, causing a complete sublimation. Even though the heavy CO₂ and H₂O molecules also break the C–C bonds at high temperature, but their impingement effect is localized and the breakage does not propagate over the entire surface.

¹This research was supported by Agency for Defence Development (ADD)

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Date submitted: 01 Aug 2014

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