グラフェンナノリボンよりカーボンアトミックチェンへの形成メカニズム

The formation mechanism from graphene nanoribbon to carbon atomic chain

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Carbon atomic chains are known to be stably bridged between two graphene terminals. They can be fabricated by electron beam thinning in a transmission electron microscope. However, the fabrication process has not been controlled due to lack of understanding of the formation process. In this study, we successfully observed the thinning process of graphene nanoribbons under low dose irradiation by spherical aberration corrected transmission electron microscope. We found that carbon atomic chains were formed when pentagons and heptagons were generated in very narrow nanoribbon (less than 1 nm in width). And the thinning processes of zigzag and armchair GNRs were found to be different. The density functional theory based molecular dynamics simulations showed that pentaheptite structure was inevitable for formation of carbon atomic chains, which was in agreement with our experimental results. Comparisons between graphene nanoribbons with zigzag and armchair edges demonstrated that the formation of CACs from zigzag GNR is more controllable.

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