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The Formation of Haeckelite Structures Induced by Vacancy Defects in Graphene Layers of Carbon Nanotube GUN-DO LEE, Seoul National University, C.Z. WANG, Iowa State University, EUIJOON YOON, NONG-MOON HWANG, Seoul National University, K.M. HO, Iowa State University, SEOUL NATIONAL UNIVERSITY COLLABORATION, IOWA STATE UNIVERSITY COLLABORATION — The formation of haeckelite structures induced by vacancy defects in graphene layers of carbon nanotube are investigated by tight-binding molecular dynamics (TBMD) simulations and by first principles total energy calculations. It is observed in the TBMD simulations that two single vacancies coalesce into a 5-8-5 double vacancy at the temperature of 3,000 K, and it is further reconstructed into a new defect structure, the 555-777 defect, by the Stone-Wales type transformation at higher temperatures. First principles calculations confirm that the 555-777 defect is energetically much more stable than two separated single vacancies, and the energy of the 555-777 defect is also slightly lower than that of the 5-8-5 double vacancy. In TBMD simulation, it is also found that the four single vacancies reconstruct into two collective 555-777 defects which is the unit for the hexagonal haeckelite structure proposed by Terrones et al. [Phys. Rev. Lett. **84**, 1716 (2000)]

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