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Migration of Carbon Adatoms on the Surface of Charged SWCNT[1] LONGTAO HAN, PREDRAG KRSTIC, State Univ of NY- Stony Brook, IGOR KAGANOVICH, Princeton Plasma Physics Laboratory — In volume plasma, the growth of SWCNT from a transition metal catalyst could be enhanced by incoming carbon flux on SWCNT surface, which is generated by the adsorption and migration of carbon adatoms on SWCNT surface. In addition, the nanotube can be charged by the irradiation of plasma particles. How this charging effect will influence the adsorption and migration behavior of carbon atom has not been revealed. Using Density Functional Theory, Nudged Elastic Band and Kinetic Monte Carlo method, we found equilibrium sites, vibrational frequency, adsorption energy, most probable pathways for migration of adatoms, and the barrier sizes along these pathways. The metallic (5,5) SWCNT can support a fast migration of the carbon adatom along a straight path with low barriers, which is further enhanced by the presence of negative charge on SWCNT. The enhancement is contributed by the higher adsorption energy and thence longer lifetime of adatom on the charged SWCNT surface. The lifetime and migration distance of adatom increase by three and two orders of magnitude, respectively, as shown by Kinetic Monte Carlo simulation. These results support the surface migration mechanism of SWCNT growth in plasma environment.

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