# §31. Creation of Chain-like Carbon Molecule by Graphene Melting

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In plasma confinement experiment [1], hydrogen plasma is poured into the divertor. The divertor is covered with carbon tiles, which is composed of graphite or carbon fiber composite. The hydrogen plasma erodes the carbon tiles and generates hydrocarbon molecules, i.e., $CH_X$, $C_2H_X$, and so on. The hydrocarbon molecules, which are regarded as dusts, interfere with the plasma confinement. Therefore, the generation of the hydrocarbon molecules should be repressed. For this purpose, we clarify how the hydrocarbon molecules are yielded by the reaction of the hydrogen plasma and the carbon tiles. It is considered that hydrogen ions catch electrons and become neutral atoms as soon as they approach the surface of the carbon tiles. The generation mechanism of the hydrocarbon molecules is derived from the investigation of the reaction of neutral hydrogen atom and graphitic material [2-4].

In the present work, we investigate the graphene melting by rise in temperature. We adopt classical molecular dynamics (CMD) simulation with modified Brenner's reactive empirical bond order (REBO) potential [2, 3, 5]. The simulation time is developed by the second order symplectic integration [6]. The time step is $5 \times 10^{-18}$ s. We set a graphene whose size is 7.87 nm $\times$ 8.52 nm with periodic boundary condition. The number of the carbon atoms is 2560. In the simulation process, the graphene temperature is raised from 300 K to target temperature by use of Nóse thermostat method [7].

Figure 1 shows that graphene melting depends on the target temperature. The melting region tends to broaden as the target temperature becomes high. In the other region of graphene, almost all six-membered cyclic structure of the graphene is saved. Moreover, chain-like carbon molecules are created in the melting region.

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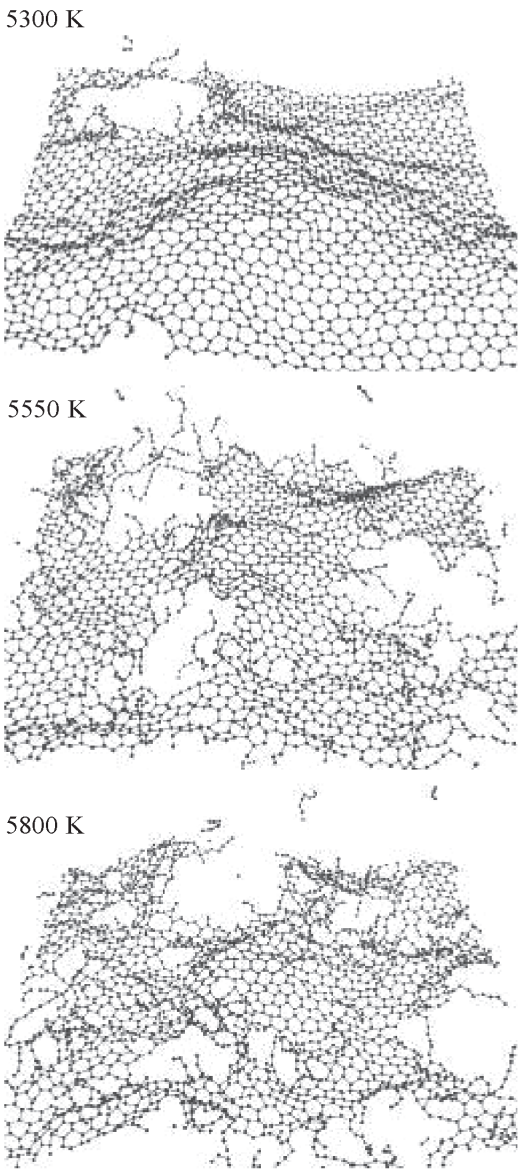


Fig. 1: The graphene melting by rise in temperature. Target temperatures of (a), (b) and (c) are set to 5300 K, 5550 K and 5800 K, respectively.

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