

## Carbon Materials with Zigzag and Armchair Edges

Yasuhiro Yamada,<sup>1</sup> Miki Kawai,<sup>1</sup> Hideki Yorimitsu,<sup>2</sup> Shinya Otsuka,<sup>2</sup> Motoharu Takanashi,<sup>3</sup> Satoshi Sato<sup>1</sup>

<sup>1</sup> Graduate School of Engineering, Chiba University, Chiba 263-8522, Japan

<sup>2</sup> Graduate School of Science, Kyoto University, Kyoto 606-8502, Japan

<sup>3</sup> Instrumental Analysis Center, Yokohama National University, Kanagawa 240-0067, Japan

Carbonization of PAHs with zigzag edges and armchair edges has been extensively studied in the past two decades. These works mentioned the presence of zigzag and armchair edges in carbonized structures, but basically only the simplified carbonized structures were exhibited, and the details are still under debate because of the difficulty to characterize the edge structures of these carbon materials without observing structures directly at atomic scale under microscopes. In this work, carbon materials with zigzag and armchair edges were prepared and the structures were determined in detail by using molecular dynamic simulation with a reactive force field (ReaxFF) to narrow down the number of possible structures and Raman spectroscopy and IR spectroscopy combined with computation. In addition, the reactivity of carbon materials with zigzag and armchair edges was compared. At the beginning, intermolecular dehydrogenation mainly proceeded because of the presence of highly reactive sites and steric hinderance. Then, intramolecular dehydrogenation proceeded despite the existence of steric hinderance, generating pentagons and the other non-hexagonal rings. As a result, two different types of carbon materials with characteristic Raman and IR spectra could be prepared. The tendency of oxidation reaction on carbonized tetracene with zigzag edges and that of carbonized chrysene with armchair edges were clearly different. Zigzag edges tended to be oxidized and increased their weight, whereas armchair edges tended to decompose without increasing their weight.