

Molecular dynamics simulation of carbon chains formation under heating of graphene nanoribbon

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Since the direct observation of carbon chain formation from graphene [1,2], their chemical, mechanical and electronic properties have attracted considerable interest. Here the method to produce carbon atomic chains by heat treatment of graphene nanoribbons (GNRs) is proposed and studied by molecular dynamics simulation. For this purpose the parameters of the first-generation bond-order Brenner potential are fitted to reproduce energies of atomic carbon chains, structures relevant for vacancy migration in graphene and three types of graphene edges. The potential with the elaborated set of parameters is applied for molecular dynamics simulations of the transformation of zigzag-edged GNRs with 3 and 4 atomic rows (3-ZGNR and 4-ZGNR) under heat treatment at 2500 K. The simulations reveal fundamentally different behaviour for 3-ZGNR and 4-ZGNR: formation of triple, double and single carbon chains with length of hundreds atoms takes place under heat treatment of 3-ZGNR, whereas for 4-ZGNR amorphization and decrease of width mainly take place at the same conditions and only short chains are observed. The atomistic mechanism of chain formation from 3-ZGNR is revealed by a detailed analysis of reactions of bond breaking and reorganization. The revealed mechanism is confirmed by comparison of the barriers of

main reactions at chains formation obtained by DFT calculations and the potential.

References

- [1] C. Jin, H. Lan, L. Peng, K. Suenaga, I. lijima, Phys. Rev. Lett., 102 (2009) 205501
- [2] A. Chuvilin, J. C. Meyer, G. Algara-Siller, U. Kaiser, New J. Phys., 11 (2009) 083019

Figures

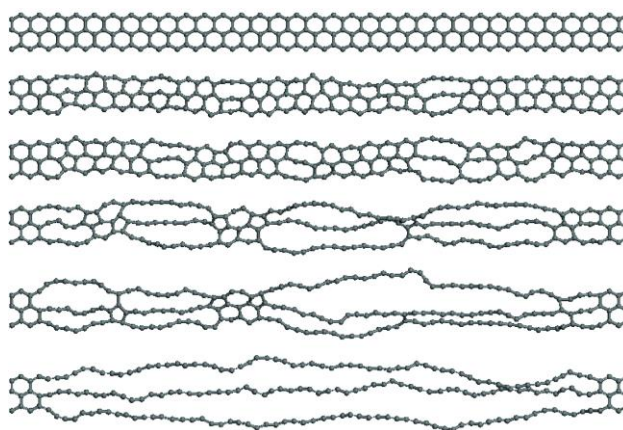


Figure 1: Simulated structure evolution of the 3-ZGNR under heating at temperature 2500 K

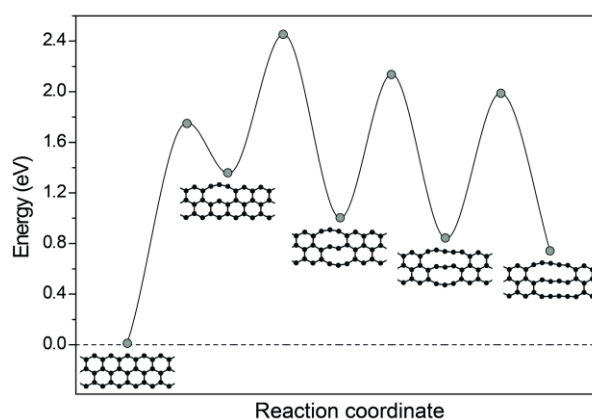


Figure 2: Schematic representation of the structure and energetics along main way of the triple parallel chain formation under heating of the 3-ZGNR