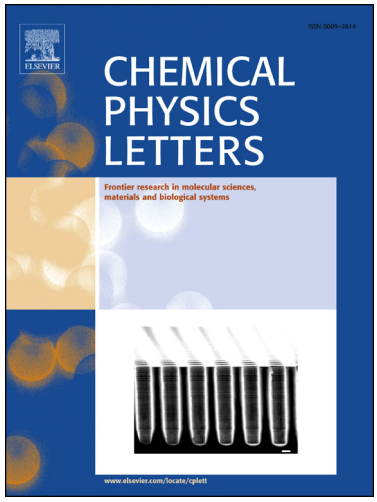

Research paper

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Molecular Dynamics Study on Core-Shell Structure Stability of Aluminum Encapsulated by Nano-carbon Materials

Qingwen Yi[1,†], Jingcheng Xu[1,†], Yi Liu[3], Dong Zhai[3], Kai Zhou[2], Deng Pan[2,*]

[1]School of Materials Science and Engineering and [2]School of Mechanical Engineering, University of Shanghai for Science and Technology, 516 Jungong Road, Shanghai 200093, China

[3]Department of Physics and Materials Genome Institute, Shanghai University, 99 Shangda Road, Shanghai 200444, China

[†]These authors contribute equally to this work.

*****Corresponding authors, E-mail: dpan@usst.edu.cn

Abstract

A ReaxFF reactive forcefield for aluminum-carbon composite system has been developed to investigate structural stability and thermal decomposition mechanism of nano-carbon materials coating aluminum particles. Research results indicated the Al@C particles were structurally stable in a broad temperature range from room temperature up to 2735K. In particular, the broken carbon cage self-healed to reconstruct a more stable Al@C core-shell structure after Al atoms sequentially departing from carbon cage during thermal decomposition, proffering an effective protection for aluminum surface-activeness.