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MOLECULAR DYNAMICS SIMULATION OF CARBON NANO-BINDERS INTO ZEOLITE THERMAL STORAGE

M. Fasano*°, M. B. Bigdeli*, M. R. Vaziri Sereshk*, E. Chiavazzo*°°, P. Asinari*

* Multi-Scale Modeling Laboratory (SMaLL - www.polito.it/small), Energy Department, Politecnico di Torino, Corso Duca degli Abruzzi, 10129 Torino, Italy
°° Chemical and Biological Engineering Department, Princeton University, Princeton, NJ, USA
° Department of Translational Imaging, The Methodist Hospital Research Institute, Houston, Texas, USA

EXTENDED ABSTRACT

In recent years, engineering nanostructures (nanowires, nanolayers and nanotubes) have attracted great attention in the development of new materials. Successful application of nanostructures requires better understanding of the emergence of normal as well as anomalous irreversible transport in such systems. Most of the times, some scales are not sufficiently well separated from the microscopic scales and, differently from the macroscopic scales, are reminiscent of the underlying reversible dynamics. Sorting out emergent continuum properties is extremely challenging. In this work, we will focus on carbon nano-binders into zeolite thermal storage as a remarkable example of such trend.

Scientists from the Fraunhofer Institute for Interfacial Engineering and Biotechnology, together with ZeoSys GmbH, have developed very recently a new type of thermal storage system [1]. This new system can store three to four times the amount of heat that water can. Moreover, it is able to store the heat loss-free over lengthy periods of time, almost indefinitely. The new system contains zeolite pellets and the key challenge is (a) to ensure optimal heat transfer (high conductivity) through the zeolite bunch during the thermal loading and (b) to ensure water percolation during the thermal release, in the same device. Recently, at Massachusetts Institute of Technology (USA), prof. Evelyn Wang is investigating carbon nano-binders (CNT, graphene and oxide graphene) surrounding the zeolite pellets, in order to meet such extreme requirements.

In the present work, we develop a simulation plan based on molecular dynamics (MD) [2] to find out the optimal functionalization of the carbon binders and the optimal density of the covalent bonds in order to build the binder matrix. The key idea is to minimize the Kapitza contact resistance between binder elements. Moreover, hybrid solutions consisting of different nano-structures (e.g. CNT and graphene) will be discussed. The most promising solutions are investigated with the aim to guide the further steps in the experimental activity.

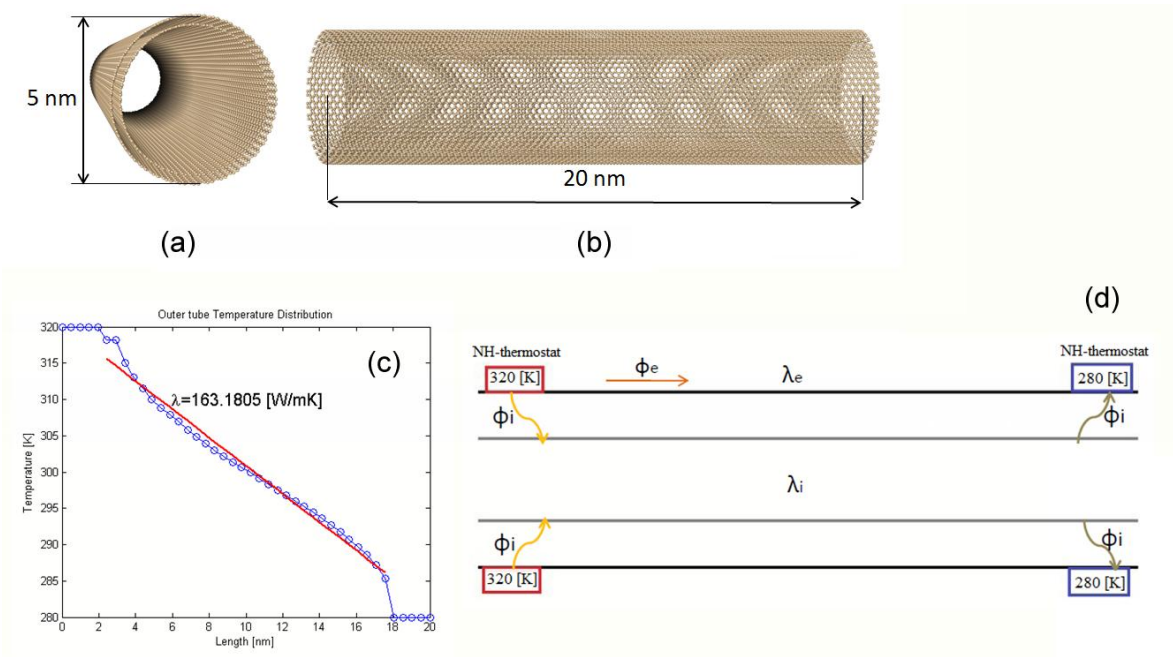

Figure 1: (a-b) Double-Walled Carbon Nano Tube (DWCNT) with chirality (33,33) and (37,37) respectively. (c) Measuring thermal conductivity by MD. (d) Schematic of the thermal power splitting between the concentric nanotubes.

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[1] Fraunhofer, Research News, Issue 06, Topic 3, 2012.
[2] D.C. Rapaport, The art of molecular dynamics simulation, Cambridge University Press, 2004.