Multiscale Hierarchical Simulation Package MULTICOMP*

A.A. Kniznik[1], R.V. Khudobin[1], D.B. Shirabaykin[1], P.V. Komarov[2,3], V.Yu. Rudyak[4], D.V. Guseva[4], P.G. Khalatur[2,3], B.V. Potapkin[1]

Kintech Lab Ltd, Moscow[1], Institute of Organoelement Compounds RAS, Moscow [2], Tver State University, Tver[3], Lomonosov Moscow State University, Moscow[4]

In recent years, significant progress has been made in the development and production of polymer/nanoparticle nanocomposites, which allows stating the appearance of nanomaterials of new generation with a wide range of applications. In many cases, these materials offer significantly improved different physicochemical properties of polymers that are attractive for wide industrial applications. The main contribution to the strength and thermal stability of nanocomposites comes from the scaffold of nanoparticles, while the conservation of the shape of the material and its plasticity are governed by the polymer matrix. The effect of nanoparticles on the macroscopic properties of polymer nanocomposites is one of the most poorly studied issues in nanosystem physics. This is because the structure of nanocomposites usually obtained experimentally is not known and they can be considered as typical "black box" systems. Such circumstance makes very important to develop verifiable models, specific simulation methods and efficient software with a view of analysis and monitoring of structure formation processes in nanomaterials. Among software packages dedicated to the calculation of physical properties of composites and multiphase materials, the most famous are the following: Materials Studio offered by Accelrys (accelrys.com), the OCTA project (octa.jp). At the moment, there is no domestic such problem-oriented software on the Russian market.

The report presents our progress of development of a hierarchical multiscale simulation package MULTICOMP. This package provides a high-level set of integrated, versatile, GUI-based tools to design, simulate and predict the morphology, thermal, mechanical, optical and electrical properties of nanoparticle-filled polymers. Nanocomposites can be simulated at different levels of spatial resolution with a possibility to transfer the data between the resolution levels in the chain "electronic structure calculation ↔ atomistic simulation ↔ mesoscopic modeling ↔ continuum theory of materials ↔ macroscopic properties".

All simulation strategies and models as part of the package are adapted to high performance parallel computing environments and can operate on currently available multi-teraflop/petaflop computational resources. It can communicate with SLURM and PBS submission systems in remote computing facilities. Parallel implementation of simulation modules depending their purpose are based on data (small molecular systems) or domain (large molecular systems) decomposition techniques. A general scheme of MULTICOMP is presented in the Figure below. It involves the following components:

(i) Combined simulation methods working at different length scales such as atomistic, coarse-grained (CG) and continual ones;

(ii) Automatic construction of CG models of molecular objects using computational schemes based on the growing neural gas algorithm and competitive Hebbian learning rules;

(iii) Innovative radical-like polymerization procedure, based on the concept of "mesoscale chemistry" for building polymer network and generating system at mesoscale level. In order to parameterize the interaction between CG particles, the iterative Boltzmann inversion method is applied;

(iv) Relaxation of the system at mesoscopic and atomistic levels;

(v) An automatic reverse mapping procedure to convert mesoscale models into atomistic representations;

* This work was carried out in the framework of the project ERA-RUS-14891 (0021028) by Kintech Lab Ltd (http://www.kintechlab.com/) with using high-performance computing resources of federal center for collective usage at NRC “Kurchatov Institute” (http://computing.kiae.ru/).

(vi) A large-scale fully atomistic molecular dynamics (MD), combined with acceleration schemes – replica-exchange MD and temperature-accelerated MD – to determine interphase properties and interfacial strengths of nanocomposite for use in higher scale models;

(vii) A continuum finite element simulation procedure for predicting the macroscopic properties of materials.

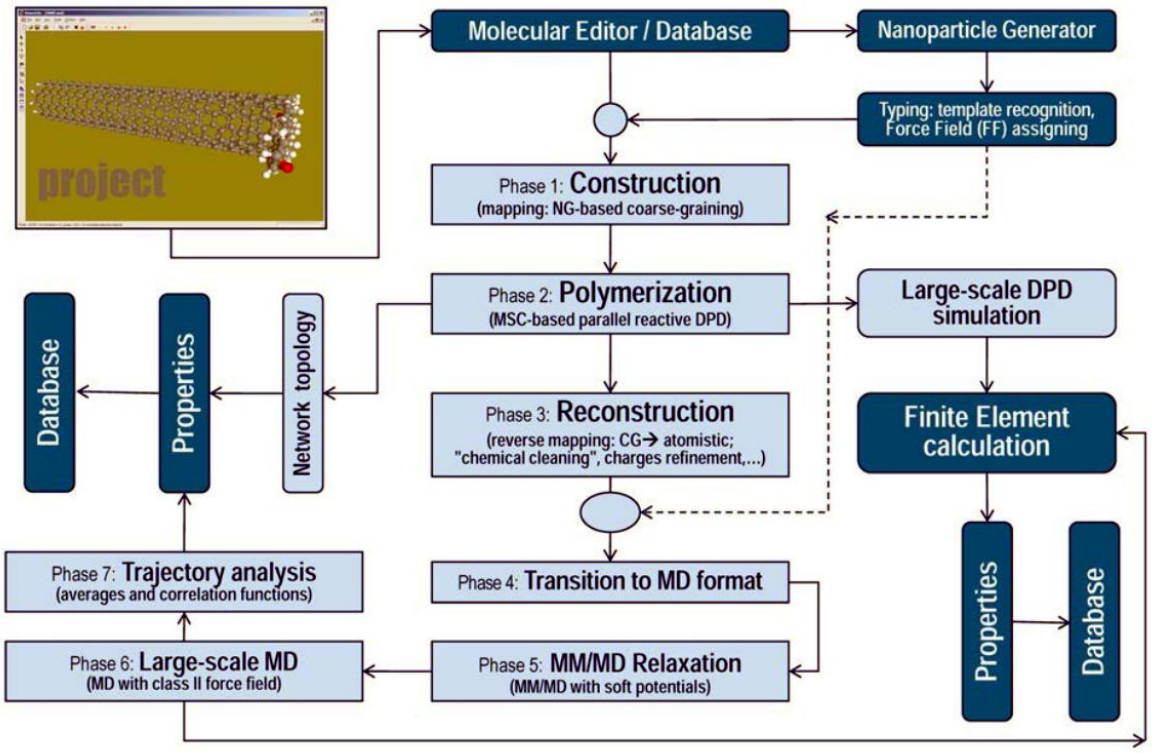

Figure. General simulation scheme of MULTICOMP.

The MULTICOMP can be used by people from different areas such as academic researchers and industrial developers. The package provides technical ability to simulate the filled polymer systems containing up to several millions of atoms using fully atomistic molecular dynamics, to simulate coarse-grained nanocomposite models on length scales up to 10 μm and for time scales up to 100 μs. As a result, researches can simulate, verify and analyze the performance of different polymer nanocomposites to evaluate the effect of different parameters on material properties, thereby improving processing recipes. In its turn, this will provide deeper insights into the complexities and the mechanics necessary to build full-scale virtual prototyping systems covering the whole design process, thus allowing engineers to get a better understanding of what is needed in the industry.

As an example of using MULTICOMP package, we also present our recent results on simulation of the effect of silica nanoparticles on the thermal and mechanical properties of thermoplastic silicone-urethane nanocomposites.

Acknowledgment. This work was carried out in the framework of a project ERA-RUS-14891 (0021028) by Kintech Lab Ltd (http://www.kintechlab.com/) with using high-performance computing resources of Federal center for collective usage at NRC “Kurchatov Institute” (http://computing.kiae.ru/).