Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Study of Polymer/Graphene Nanocomposites through Atomistic Molecular Dynamics Simulations ANASTASSIA RISSANOU, Institute of Applied and Computational Mathematics (IACM), Foundation for Research and Technology Hellas (FORTH), GR-71110 Heraklion, Crete, Greece, VAGELIS HARMANDARIS, Department of Applied Mathematics, University of Crete, GR-71409, Heraklion, Crete, Greece — Polymer/graphene nanostructured systems have attracted great attention the last years both for scientific and technological reasons. A main challenge in the study of graphene based polymer nanocomposites is to predict their properties at the molecular level. In the current study the effect of the weight fraction of graphene in a polymer matrix, as well as the size of the graphene sheet, on the properties of polymer chains are examined. Density profiles, structural and conformational characteristics as well as mobility aspects are studied. All the above properties are examined, as a function of the distance from the substrate. Results are compared with the interfacial properties of polymer chains confined between two periodic (i.e., "infinite") frozen graphene layers. In addition dynamical and conformational properties of the graphene sheet are studied as a function of the size and the weight fraction of the sheet in the polymer matrix. Furthermore, thermal as well as matrix induced fluctuations (i.e. wrinkling) of graphene sheets are examined. The extent of the fluctuations and the frequency of conformation interchange between crests and troughs are computed. All above properties are presented for different polymeric systems.

Anastassia Rissanou
Institute of Applied and Computational Mathematics (IACM),
Foundation for Research and Technology Hellas (FORTH),
GR-71110 Heraklion, Crete, Greece

Date submitted: 14 Nov 2014 Electronic form version 1.4