11th World Congress on Computational Mechanics (WCCM XI)
5th European Conference on Computational Mechanics (ECCM V)
6th European Conference on Computational Fluid Dynamics (ECFD VI)
July 20 - 25, 2014, Barcelona, Spain

# COMPUTATIONAL MODELLING OF THE COMPRESSIVE BEHAVIOUR OF CNT-REINFORCED ALUMINIUM COMPOSITES

**Nuno Silvestre [1], Bruno Faria[2] and José N. Canongia Lopes [3]**

[1] Dept. Mechanical Engng, IST, Univ. Lisbon, Av. Rovisco Pais, 1049-001 Lisboa, Portugal
nsilvestre@ist.utl.pt
[2] Dept. Mechanical Engng, IST, Univ. Lisbon, Av. Rovisco Pais, 1049-001 Lisboa, Portugal
[3] Dept. Chemical Engng, IST, Univ. Lisbon, Av. Rovisco Pais, 1049-001 Lisboa, Portugal

**Key Words:** *Nanocomposites, Computational methods, Nanotubes, Mechanical properties*

This paper presents a Molecular Dynamics (MD) study on the characterization of the compressive behavior of an aluminium (Al) material reinforced with carbon nanotubes (CNTs). Firstly, a detailed literature review of recent experimental and numerical works dedicated to the characterization and mechanical enhancement of CNT-Al composites is presented. Then, the paper describes a computational approach based on MD simulations used to analyze the mechanical behavior of the CNT-Al composite material under compression. Finally, the paper presents and discusses several results that comprise (i) curves relating the energies (total, Al, CNT, interface) with the imposed axial shortening displacement, (ii) plots of deformed shapes and failure modes of CNT-Al specimen and (iii) curves relating the acting stress with the imposed strain. In this study, we adopted two limit cases for bonding between the CNT and Al matrix, one in which the displacements are imposed to the Al atoms (case A) and another in which displacements are imposed to both Al and C atoms (case B). In comparison with pure Al, the Young's modulus increases about 50% in case A and 100% in case B. These increases are not only due to the CNT intrinsic stiffness but also to the interface slip stresses, which are about 16 MPa (case A) and 75 MPa (case B). In opposition, it is seen that both yield stress and yield strain do not increase. This evidence is mostly due to premature failure of the CNT-Al composite due to CNT local buckling. This study not only confirms previous results obtained by other researchers but also provides some understanding on the compressive behavior of CNT-based composites, which might be different to standard tensile behavior.

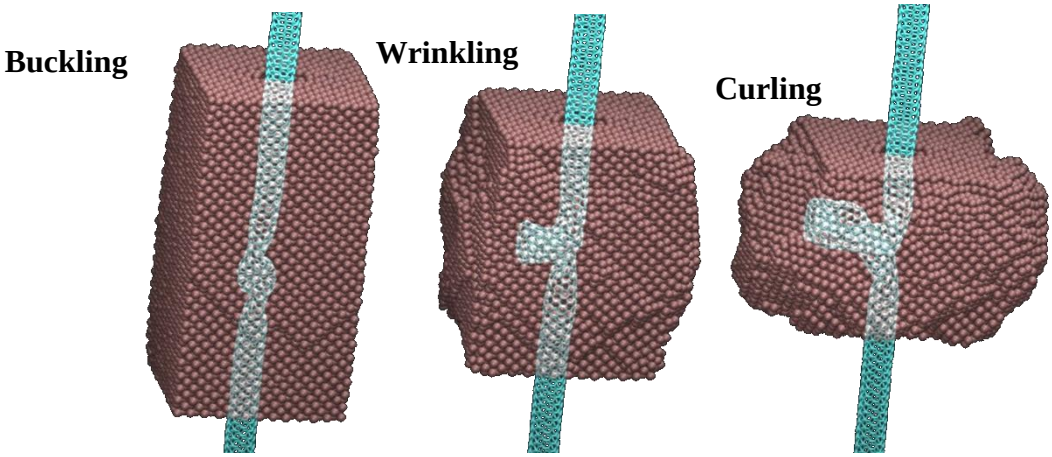


**Figure 1**. Deformed configurations of CNT-reinforced aluminium sample.