Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Analysis of the Behaviour of Nanocomposites by Multi-scale Simulation[1] WOONG LEE[2], Yonsei University, WOO-SUNG JUNG, Korea Advanced Institute of Science and Technology, JAE-MIN MYOUNG, Yonsei University
— Hierarchical multi-scale simulation scheme was introduced for the analysis of the mechanical behaviour of nanocomposites. Aluminium matrix composites reinforced with uniformly dispersed carbon nanotube (CNT) was chosen as a model system. Ab initio simulation was first carried out to estimate inter-atomic potential between a CNT and an Al atom and to determine type of bonding between CNT and Al. This fundamental information was then passed onto the molecular dynamic (MD) simulation in which the interface properties between the matrix and the reinforcement was characterised in terms of load-displacement behaviour by simulating a CNT pullout test. Continuum analysis wad carried out with this interface properties to finally extract representative properties of CNT-reinforce Al matrix nanocomposites using representative volume element approach. Fracture behaviour was also estimated by analysing possible crack paths within the nanocomposites.

[1]This work was supported in part (WL and JMM) by the Korea Research Foundation Grant funded by Korean Government (MOEHRD) R08-2004-000-10193-0.
[2]Corresponding author

Woo-Sung Jung
Korea Advanced Institute of Science and Technology

Date submitted: 29 Nov 2005 Electronic form version 1.4