Due to its high stiffness, carbon nanotubes (CNTs) are considered as one of the widely used reinforcement materials in the metal matrix composites. In this thesis, finite element (FE) models were built in Ls-Dyna3D to simulate Copper/CNTs composite deformation and fracture, and to explore CNTs reinforcement mechanisms. Several possible mechanisms were discussed.

Deformation and failure of Cu/CNT composites were studied numerically using unit cell FE models, which consist of both metal matrix and CNTs. The simulation results have been verified by existing experiment data reported by Chen's group. The matrix material was modeled as elasto-plastic ductile solids. The CNTs material properties were taken from literature results using molecular dynamics simulation. FE simulations have showed that CNTs deformation exceeds material elastic limit, which means that CNTs plasticity should be taken into account as well. 2D unit cell models were developed using axial symmetric elements with suitable boundary conditions. Several mechanisms are found to affect CNTs reinforcement prediction. The first one is the boundary condition imposed in the models. The CNTs significantly affect the plastic flow of copper during plastic deformation, which is one important reinforcement mechanism. The second reinforcement mechanism is found to be the hardening zone of Cu matrix around CNTs, which is introduced by mismatch of coefficient of thermal expansion (CTE).

A round of parametric studies was performed to investigate the effects of several modeling parameters in the FE simulations; these parameters include the volume fraction of CNTs, aspect ratio of CNTs, the size of hardening zone, and the residual plastic strain in the zone. A tool combining Matlab and Ls-Dyna was developed to automatically build 2D unit cell models and automatically post-process simulation results. Picking up suitable parameters, 2D unit cell model results well predict the experimental results from Chen's group. It should be noted that the interface between Cu and CNTs was assumed to be perfect in FE simulations since no CNTs debonding was observed in the experiments.

Also, a 3D unit cell model using tetrahedral elements (with element numbers up to one million) was tentatively developed to obtain more accurate results. The purpose was to explore the interface properties of Cu/CNTs, the effect of CNTs orientation distribution, and the other reinforcement mechanism coming from geometry necessary dislocation (GND) since the size of Cu matrix is divided into nano scales by CNTs. 3D unit models are also used to verify the 2D unit cell one, which is a simplified and effective approach. Very interesting results was observed in this part of study. Further works are needed to overcome the difficulties in 3D modeling and the limitation of current CPU speed.