Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Atomic Nanotube Welders. MORINOBU ENDO, HIROYUKI MURAMATSU, TAKUYA HAYASHI, YOONG-AHM KIM, Shinshu University, Japan, GREGORY VAN LIER, JEAN-CHRISTOPHE CHARLIER, Université Catholique de Louvain, Belgium, HUMBERTO TERRONES, IPICYT, Mexico, MILDRED S. DRESSELHAUS, MIT, USA, MAURICIO TERRONES, IPICYT, Mexico — We demonstrate that the incorporation of boron between double walled carbon nanotubes (DWNTs) during thermal annealing results in covalent nanotube "Y" junctions, DWNT coalescence and the formation of flattened multi-walled carbon nanotubes (MWNTs). The processes occur via the merging of adjacent tubes which is triggered by B interstitial atoms. In order to demonstrate the unique welder properties of B in the process, we have carried out *AM1* molecular dynamics simulations at high temperatures and *ab-initio* calculations. We observe that B atom interstitials between DWNTs are responsible for the rapid establishment of covalent connections between neighboring tubes (polymerization). Once B is in the lattice, tube faceting (polygonization) starts to occur, and the electronic properties are expected to change dramatically.

Mauricio Terrones
IPICYT, Mexico

Date submitted: 03 Dec 2005 Electronic form version 1.4