Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Study of metal oxide nanostructures using molecular dynamics simulation WUN CHET DAVY CHEONG, Institute of Materials Research and Engineering, A*STAR — The nanostructures of metal oxides such as TiO2 and ZnO have a wide range of potential applications such as in catalyst, photoelectronics, photochemistry, surface coatings and power generation. However, experimental methods to characterize these nanostructures are limited and the growth mechanisms of these nanostructures are still not well understood. In this study, molecular dynamics is used to elucidate some interesting mechanical properties of TiO2 and ZnO nanowires on a size scale that is currently still not possible to investigate experimentally. It is found that the mechanical properties of these nanowires vary drastically and differently depending on the size of the wires. Classical molecular dynamics is able to clearly explain the different mechanisms and their causes. Simulation results show that while large surface-to-volume ratio is responsible for their size effects, ZnO and TiO2 wires displayed opposite trends. It was also found that when crystalline ZnO nanowires are stretched, necking initiated at localized amorphous regions to eventually form single-atom chains which can sustain strains above 100%. Such large elongations are not observed in TiO2 nanowires. Molecular dynamics is also used to explain the formation of nanorings, helices and bows by ZnO nanobelts.

Wun Chet Davy Cheong
Institute of Materials Research and Engineering, A*STAR

Date submitted: 30 Nov 2009 Electronic form version 1.4