Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

The Structure, Stability and Origin of beta-Phase Ta AIQIN JIANG[1], TREVOR TYSON[2], LISA AXE[3], New Jersey Institute of Technology —
Tantalum thin films exhibit two crystalline phases, bcc (α-phase, the bulk structure of tantalum) and metastable tetragonal β-phase, which differ in both mechanical and electrical properties. In order to understand the stability of the β phase and the origin of the β-to-α phase transformation, molecular dynamics simulations have been performed on tantalum clusters. Molecular dynamics simulations show that the β phase is stable with a very high melting point. No phase transformation was observed for pure β-Ta clusters from room temperature to the melting point. Simulations of Ta clusters with mixed α and β phases revealed that inclusion of a small α-Ta cluster inside a β-Ta cluster induces β to bcc transformation at a temperature far below its melting point, depending on the cluster size and α to β atom ratio. These results suggest that the observed β to bcc transformation results from the presence of small α-phase grains within the β-Ta films. The growth of β-Ta on substrate as a result of strain is being evaluated.

[1]Department of Physics
[2]Department of Physics
[3]Department of Civil and Environmental Engineering

Aiqin Jiang
New Jersey Institute of Technology

Date submitted: 23 Nov 2004 Electronic form version 1.4