Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Superheating, Melting and Precursors to Melting in Metal Nanoparticles DMITRI SCHEBARCHOV, Victoria University of Wellington, SHAUN HENDY, Industrial Reseach Ltd — We have investigated precursors to melting in metal nanoparticles using molecular dynamics in the microcanonical ensemble. At the onset of solid-liquid phase coexistence, we find first-order transitions in clusters with non-melting facets (i.e. facets that are not wet by the melt such as Pb (111)), and continuous transitions otherwise. In sufficiently small clusters however, we find that static solid-liquid coexistence is unstable. Further, the size at which the instability arises, and even the melting temperature, depends on the ability of the melt to wet the solid facets of the cluster. In particles with non-melting facets we show that the melting temperature can exceed that of the bulk material. Finally, we also discuss a range of solid-solid transitions that have been observed to occur during solid-liquid phase coexistence, some of which are again driven by the preference of the melt to wet certain crystal facets.

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Date submitted: 07 Feb 2008 Electronic form version 1.4