Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Deformation twinning activated $\alpha \rightarrow \omega$ transformation in titanium under shock compression. HONGXIANG ZONG, TURAB LOOKMAN, Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA — Materials dynamics, especially the behavior of solids under extreme compression, is a topic of broad scientific and technological interest. However, less is known of the role of grain boundary structures on the shock response of hexagonal-close-packed metals. We use molecular dynamics simulations to study deformation mechanisms in shock compressed Ti bicrystals containing three types of grain boundary (GB) microstructures, i.e., coherent twin boundaries (CTBs), symmetric incoherent twin boundaries (ITB) and {1-210}asymmetric tilt grain boundaries. Our results show that both dislocation activity and the $\alpha \rightarrow \omega$ phase transformation in Ti are sensitive to the GB characteristics. In particular, we find that the elastic shock wave can readily trigger the $\alpha \rightarrow \omega$ transformation at CTBs but not at the other two GBs, and the activation of the $\alpha \rightarrow \omega$ transformation at CTBs leads to considerable wave attenuation (i.e., the elastic precursor decay). Combined with first principle calculations, we find that CTBs can facilitate the overcoming of the energy barrier for the $\alpha \rightarrow \omega$ transformation. Our findings have potential implications for interface engineering and materials design under extreme conditions.

Turab Lookman
Los Alamos Natl Lab

Date submitted: 04 Nov 2015 Electronic form version 1.4