Abstract Submitted for the MAR07 Meeting of The American Physical Society

Phonon-based Mechanisms for Structural Transformations in Pu TURAB LOOKMAN, AVADH SAXENA, ROBERT ALBERS, Los Alamos National Laboratory — Plutonium undergoes a number of transformations that involve changes in unit cell shape and numbers of atoms. We focus on the fcc to monoclinic $\delta \to \alpha'$ transformation and suggest displacive mechanisms that can describe the transformation. We also explore signatures of the mechanisms in phonon dispersion curves and present a phase diagram in paramter space. The implications for the $\beta \to \alpha$ transformation, assuming a displacive mechanism, will also be explored.

Turab Lookman Los Alamos National Laboratory

Date submitted: 20 Nov 2006 Electronic form version 1.4