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 parameter space. The implications for the $\beta \to \alpha$ transformation, assuming a displacive mechanism, will also be explored.