Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

First-principles elastic constants and phonons of δ-Pu PER SÖDERLIND, ALEX LANDA, BABAK SADIGH, Lawrence Livermore National Laboratory, PHYSICS DEPARTMENT TEAM — Elastic constants and zone boundary phonons of δ-Pu have been calculated within the density-functional theory. The electronic structure is modeled by disordered magnetism utilizing either the disordered local moment or the special quasi-random structure techniques. The anomalously soft C^{prime} as well as a large anisotropy ratio of δ-Pu is reproduced by this first-principles model. Also the measured phonons for δ-Pu compare relatively well with their theoretical counterpart at the zone boundary.

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Date submitted: 07 Dec 2004 Electronic form version 1.4