UZr-Nd paper

Performing scoping study with ispin1, ispin2, ispin2+U

Dopants:

Pd, Sn, As, Se – maybe not Se

Fission products:

Nd, Ce

Data

Formation energies of point defects of each of these dopants

Formation energies of point defects of each of these FPs

Binding energies of Dopant to FP

Binding energy of Dopant to vac

Binding energy of FP to vac

Binding energy of Dopant to Zr

Binding energy of FP to Zr

All binding energies taken at three points: (each 1nn), as well as two longer distance points

Diffusion not necessary:

This tells:

Energetic relationship of FPs with Dopants and with Zr, which indicates propensity to form clusters

Binding with vacancies shows ability to diffuse