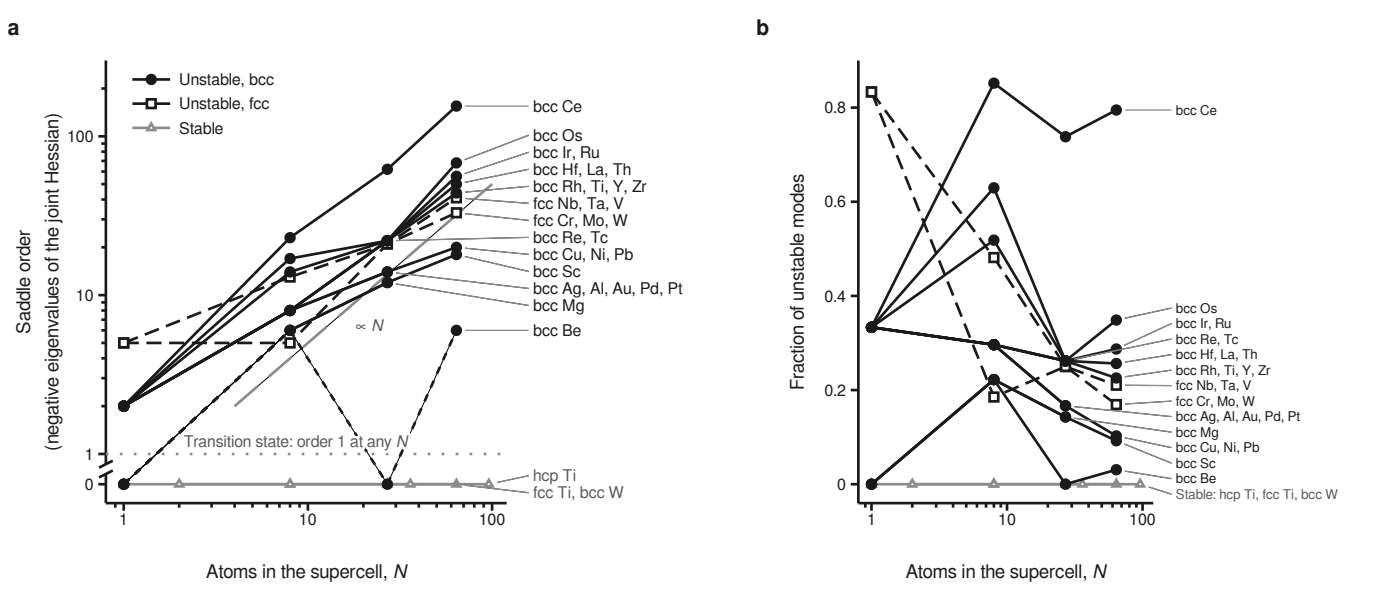
a
Unstable, bcc
Unstable, fcc
Stable
Saddle order
(negative eigenvalues of the joint Hessian)
100
10
1
0
1
10
100
Atoms in the supercell, N
bcc Ce
bcc Os
bcc Ir, Ru
bcc Hf, La, Th
bcc Rh, Ti, Y, Zr
fcc Nb, Ta, V
fcc Cr, Mo, W
bcc Re, Tc
bcc Cu, Ni, Pb
bcc Sc
bcc Ag, Al, Au, Pd, Pt
bcc Mg
bcc Be
∝ N
Transition state: order 1 at any N
hcp Ti
fcc Ti, bcc W
b
Fraction of unstable modes
0.8
0.6
0.4
0.2
0
1
10
100
Atoms in the supercell, N
bcc Ce
bcc Os
bcc Ir, Ru
bcc Re, Tc
bcc Hf, La, Th
bcc Rh, Ti, Y, Zr
fcc Nb, Ta, V
fcc Cr, Mo, W
bcc Ag, Al, Au, Pd, Pt
bcc Mg
bcc Cu, Ni, Pb
bcc Sc
bcc Be
Stable: hcp Ti, fcc Ti, bcc W