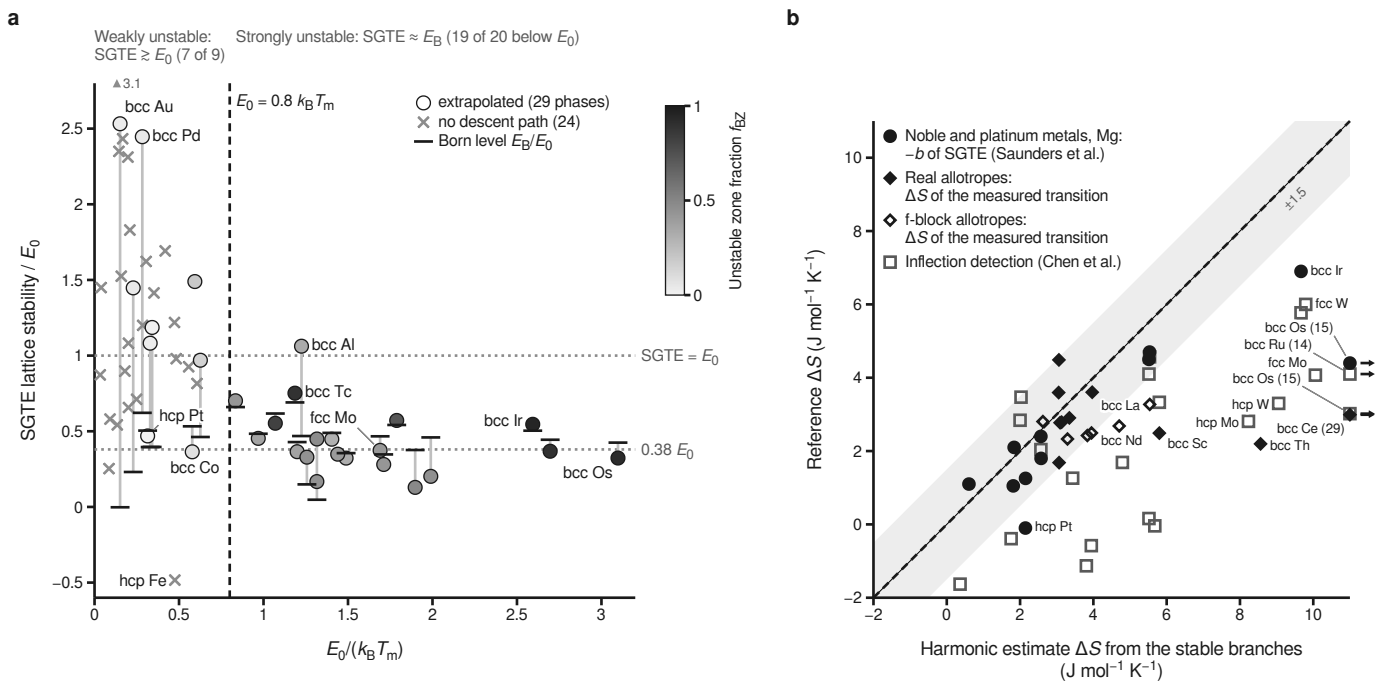
a
Weakly unstable:
SGTE ≳ E_0 (7 of 9)
Strongly unstable: SGTE ≈ E_B (19 of 20 below E_0)
▲3.1
bcc Au
bcc Pd
$E_0 = 0.8\ k_B T_m$
extrapolated (29 phases)
no descent path (24)
Born level E_B/E_0
Unstable zone fraction f_{BZ}
1
0.5
0
bcc Al
SGTE = E_0
bcc Tc
fcc Mo
hcp Pt
bcc Ir
0.38 E_0
bcc Co
bcc Os
hcp Fe
SGTE lattice stability / E_0
$E_0/(k_B T_m)$
b
Noble and platinum metals, Mg:
−b of SGTE (Saunders et al.)
Real allotropes:
ΔS of the measured transition
f-block allotropes:
ΔS of the measured transition
Inflection detection (Chen et al.)
±1.5
bcc Ir
fcc W
bcc Os (15)
bcc Ru (14)
fcc Mo
bcc Os (15)
hcp W
hcp Mo
bcc Ce (29)
bcc Th
bcc La
bcc Nd
bcc Sc
hcp Pt
Reference ΔS (J mol^{-1} K^{-1})
Harmonic estimate ΔS from the stable branches
(J mol^{-1} K^{-1})