Computational Materials Physics

Center for Molecular Modeling

Department of Materials Science and Engineering

composition-dependent ground state phase diagrams

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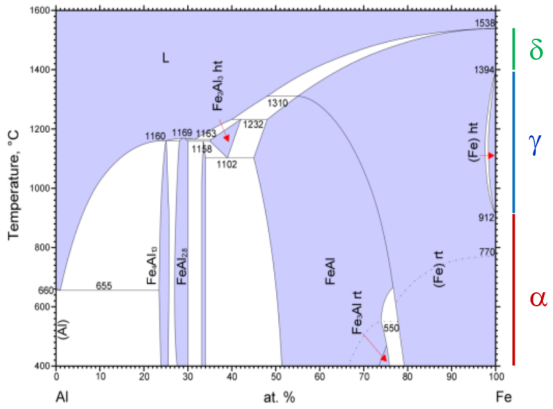
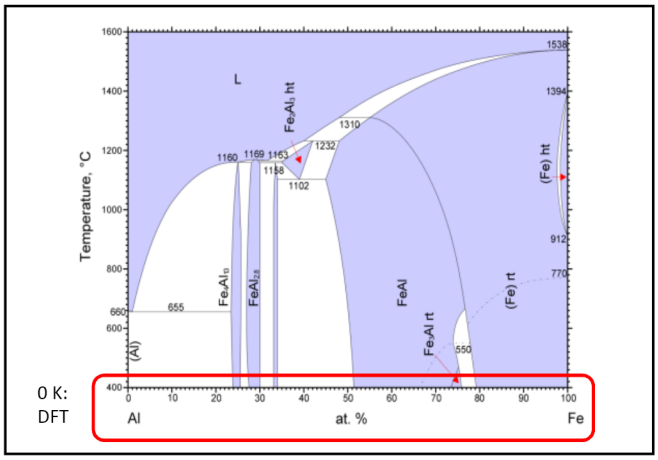
http://molmod.ugent.be
http://www.ugent.be/ea/dmse/en
my talks on Youtube: http://goo.gl/P2b1Hs

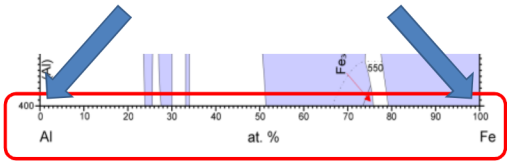




cohesive energy

$$E_{coh} = E_{solid} - E_{atom}$$

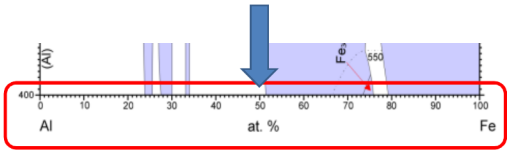
Is solid fcc Al energetically stable ?
Is solid bcc Fe energetically stable ?



formation energy

$$E_{form} = E_{alloy} - (E_{solid\text{-}1} + E_{solid\text{-}2})$$

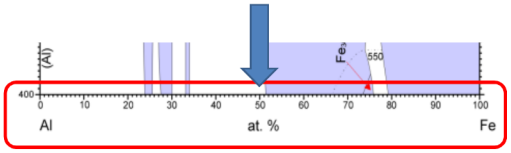
Is solid CsCl-FeAl energetically stable ?

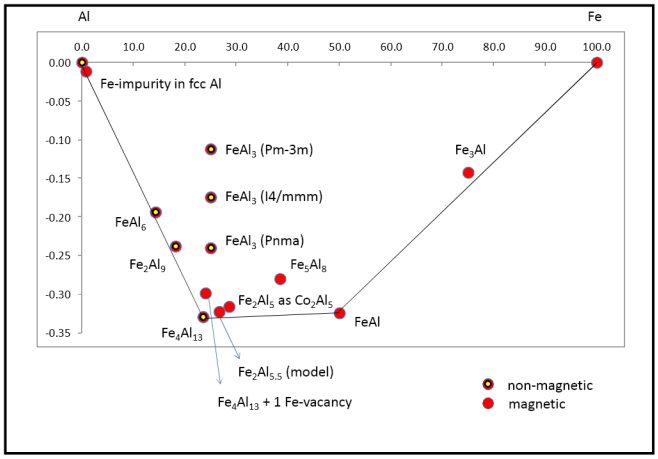


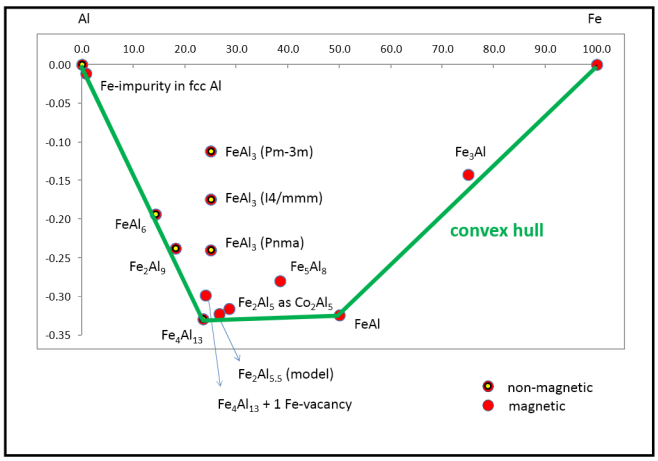
formation energy

$$E_{form} = E_{alloy} - (E_{solid\text{-}1} + E_{solid\text{-}2})$$
$$= E_{CsCl\text{-}FeAl} - (E_{fcc\text{-}Al} + E_{bcc\text{-}Fe})$$

Is solid CsCl-FeAl energetically stable ?




Al
Fe
0.0 10.0 20.0 30.0 40.0 50.0 60.0 70.0 80.0 90.0 100.0
0.00 -0.05 -0.10 -0.15 -0.20 -0.25 -0.30 -0.35
Fe-impurity in fcc Al
FeAl3 (Pm-3m)
Fe3Al
FeAl3 (I4/mmm)
FeAl6
FeAl3 (Pnma)
Fe2Al9
Fe5Al8
Fe2Al5 as Co2Al5
FeAl
Fe4Al13
Fe2Al5.5 (model)
Fe4Al13 + 1 Fe-vacancy
non-magnetic
magnetic


Al
Fe
0.0 10.0 20.0 30.0 40.0 50.0 60.0 70.0 80.0 90.0 100.0
0.00 -0.05 -0.10 -0.15 -0.20 -0.25 -0.30 -0.35
Fe-impurity in fcc Al
FeAl3 (Pm-3m)
Fe3Al
FeAl3 (I4/mmm)
convex hull
FeAl6
FeAl3 (Pnma)
Fe2Al9
Fe5Al8
Fe2Al5 as Co2Al5
FeAl
Fe4Al13
Fe2Al5.5 (model)
Fe4Al13 + 1 Fe-vacancy
non-magnetic
magnetic