Elastic properties of $Al_xCrMnFeCoNi$ high-entropy alloys from *ab initio* theory

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Introduction

High-entropy alloys (HEAs)

- Definition: HEAs=A+B+C+D+E+… && 5%<A\B\C\D\E\...<35%
- Excellent mechanical properties (e.g. CrMnFeCoNi)
- Alloying effect $Al_xCrMnFeCoNi$

EMTO-CPA

Introduction

Single Crystal Elastic Constants

$$c_{ijkl} = \frac{1}{V}\frac{\partial E}{\partial e_{ij}\partial e_{kl}}$$

$$B(V) = V\frac{\partial^2 E(V)}{\partial V^2}$$

C' C_{44}

B

$$C' = \frac{C_{11} - C_{12}}{2}$$

$$B = \frac{C_{11} + 2C_{12}}{3}$$

Introduction

$$E = 9BG/(3B+G)$$

$$v = (3B\text{-}2G)/(6B+2G)$$

Polycrystalline Elastic Constants

Voigt

$$B_V = \frac{C_{11} + 2C_{12}}{3}$$

$$G_V = \frac{C_{11} - C_{12} + 3C_{44}}{5}$$

Reuss

$$B_R = \frac{C_{11} + 2C_{12}}{3}$$

$$G_R = \frac{5(C_{11} - C_{12})C_{44}}{4C_{44} + 3(C_{11} - C_{12})}$$

Hill

$$B_H = \frac{1}{2}(B_V + B_R)$$

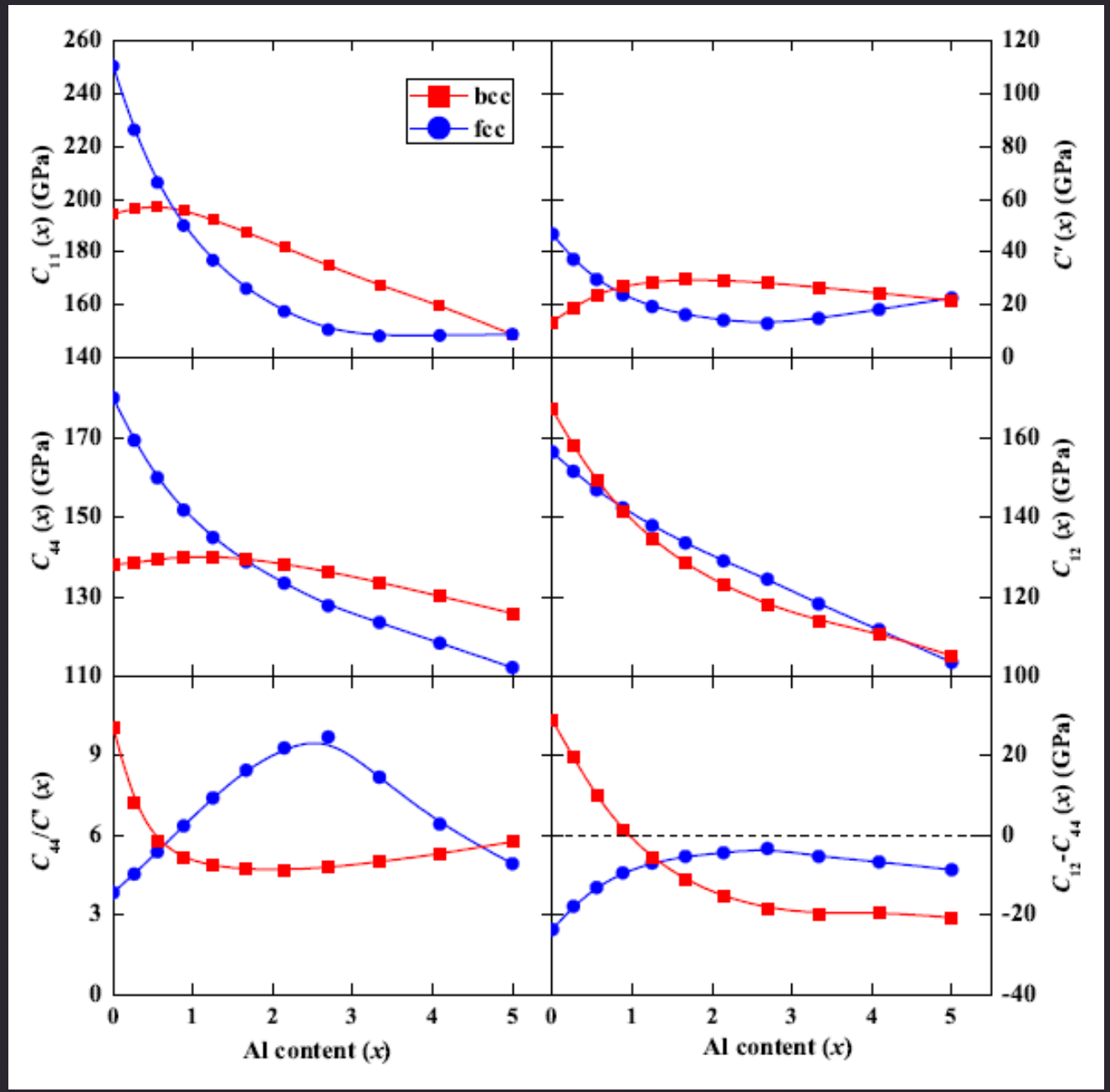
$$G_H = \frac{1}{2}(G_V + G_R)$$

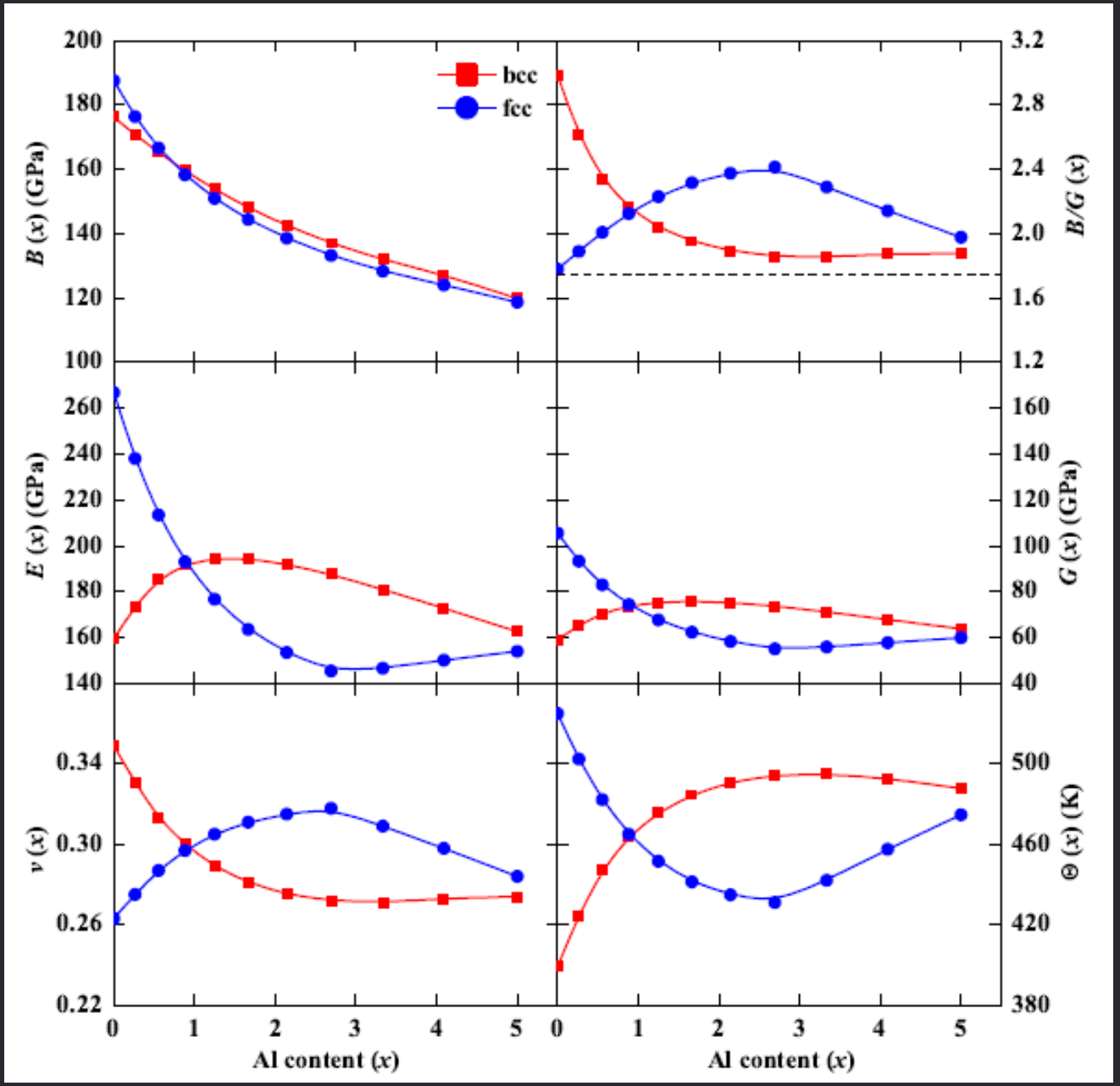
Results

Single Crystal Elastic Constants

$Al_xCrMnFeCoNi$

PBE-PBE **Soft-core**

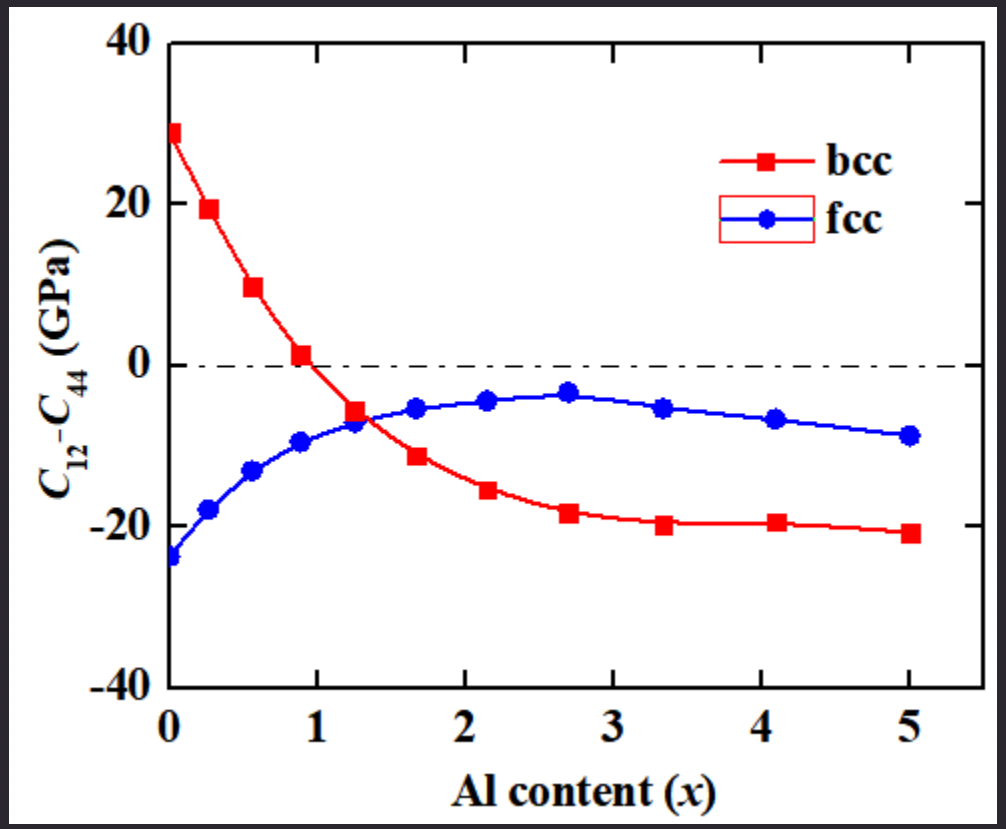




Polycrystalline Elastic Constants

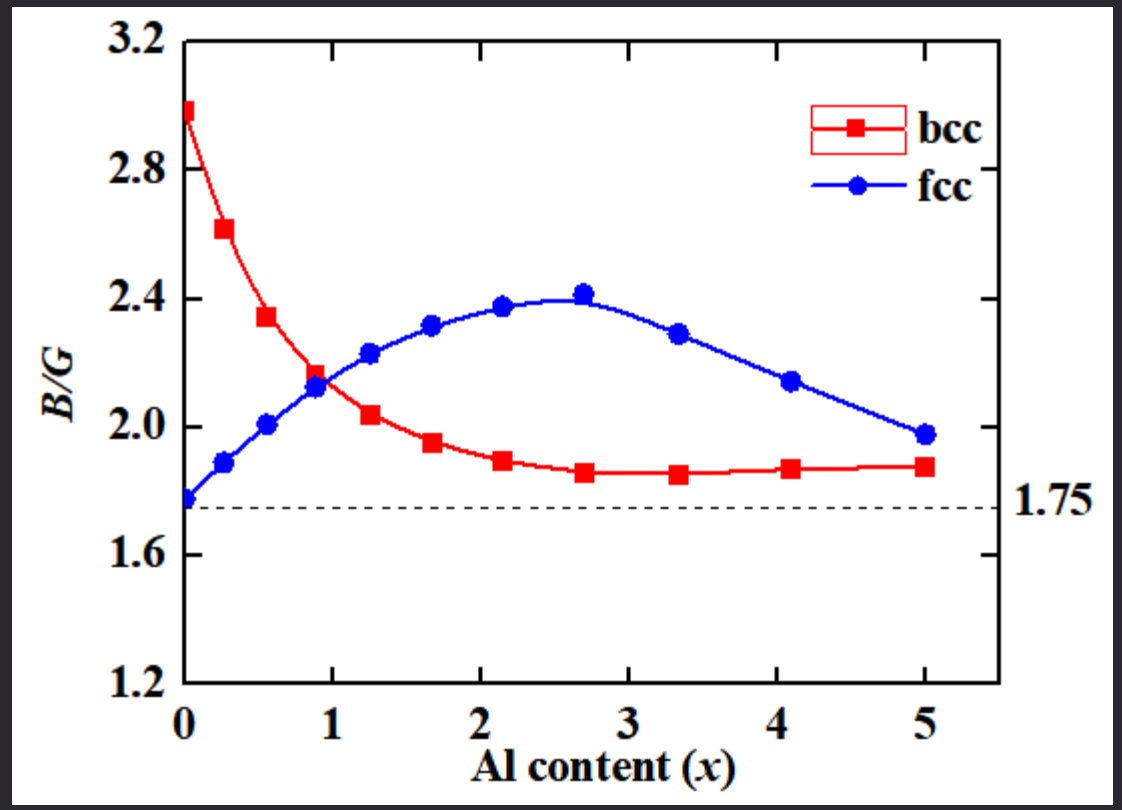
$Al_xCrMnFeCoNi$

Discussion



Ductile

Brittle



Cauchy pressure $CP=C_{12}-C_{44}$

Pugh ratio B/G

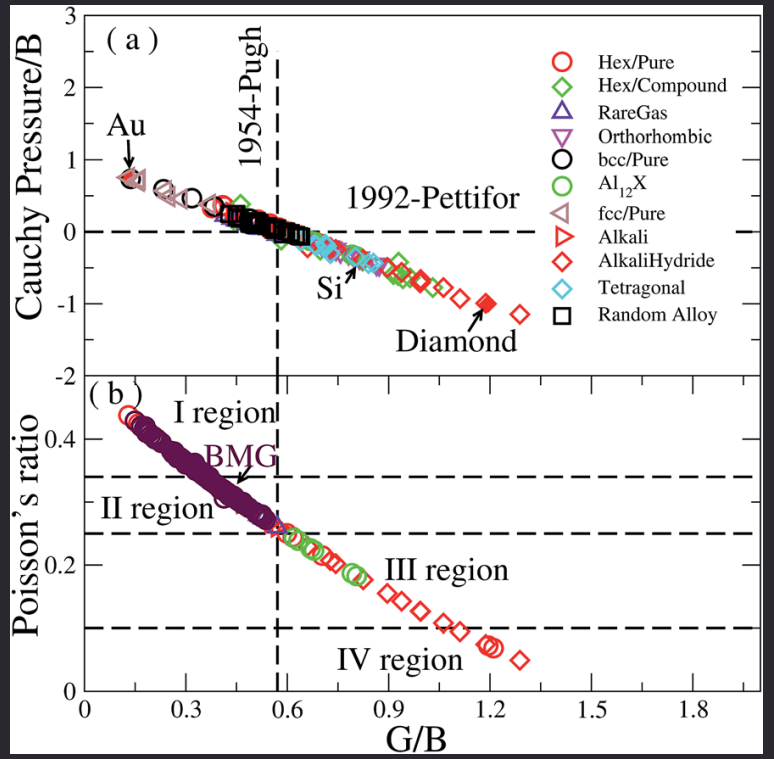
Discussion

Pugh ratio B/G

Cauchy pressure $CP=C_{12}-C_{44}$

Voigt $$\frac{B_V}{G_V} = \frac{C_{11} + 2C_{12}}{3} \frac{5}{C_{11} - C_{12} + 3C_{44}}$$

$C_{12}-C_{44}=B_V-5/3G_V$



CP/B* as a function of *G/B

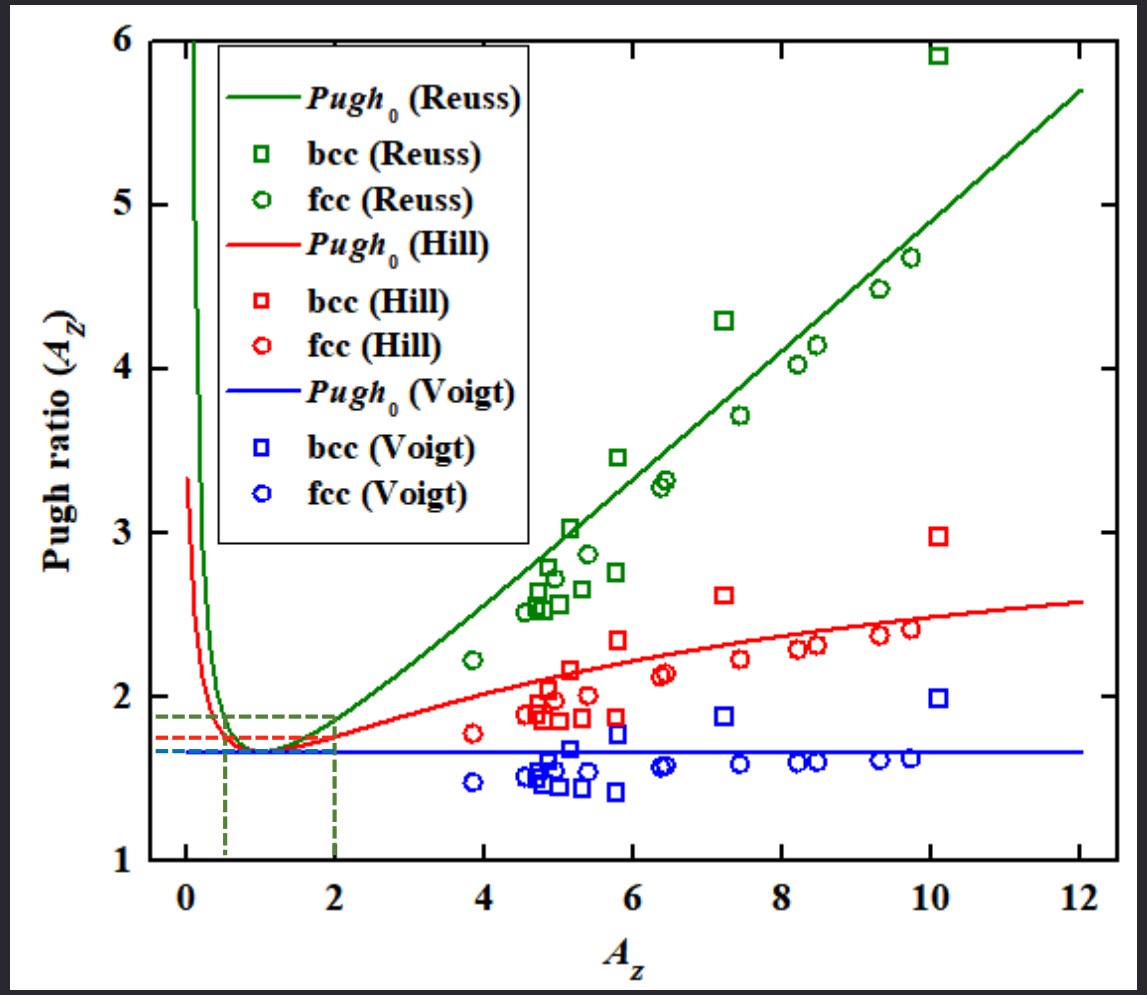
(Wang et al. RSC Adv., 2016, 6, 44561)

$CP= 0.995B-1.620G$

Discussion

- Empirical — Cauchy pressure (CP_0=0) — Pugh ratio criterion ($Pugh_0$=1.75)
- Voigt — C_{12}-C_{44}=B_V-5/3G_V — CP_0=0 — $Pugh_0$=1.67
- Reuss — $Pugh_0^R(A) = \frac{1}{15}\left(\frac{6}{A} + 13 + 6A\right)$ — Zener anisotropy A=C_{44}/C'
- Hill — $Pugh_0^H(A) = \frac{10}{3}\frac{1}{\frac{25}{\frac{6}{A} + 13 + 6A} + 1}$

Discussion



$Pugh_0$ as a function of A_z (C_{12}-C_{44} =0)

Alloy	CP	B/G	AZ
Fe	35.2	2.1	1.4
CrMoTiV	61.3	2.46	0.73
MoNbTiV	60.9	2.54	0.9
$Fe_{0.97}Mn_{0.03}$	12.01	1.82	1.42
$Fe_{0.9}Mn_{0.1}$	-6.71	1.64	1.55
$Fe_{0.97}Ni_{0.03}$	34.4	2.09	1.36
$Fe_{0.9}Ni_{0.1}$	55.9	2.43	1.83

Phys. Rev. B 79 (2009) 224201
Comput. Mater. Sci. 128 (2017) 185–190
Phys. Rev. B 91 (2015) 224203

Discussion

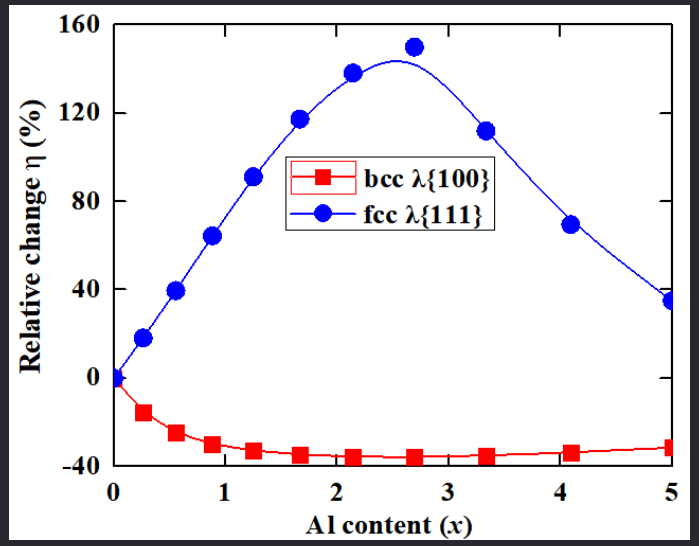
Theoretical cleavage stress

$$\sigma_{cl.}\{lmn\} = \left(\frac{E_{lmn}\gamma_{lmn}}{d_{lmn}}\right)^{1/2}$$

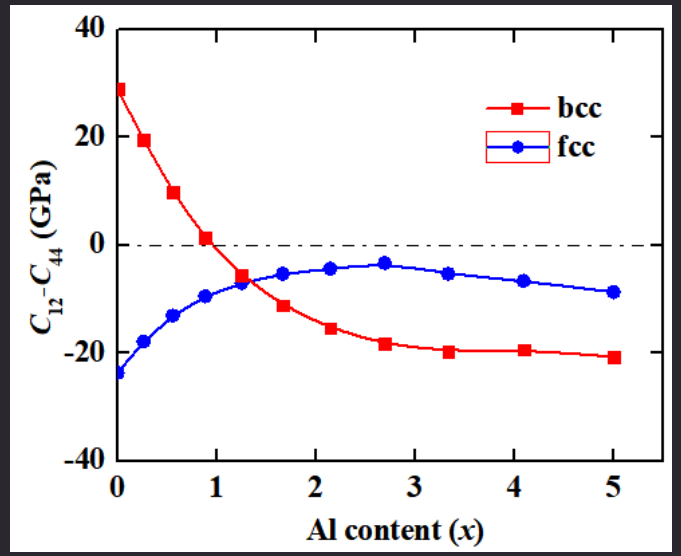
bcc $\lambda\{110\} \equiv \sigma_{cl.}\{110\}/G\{110\}\langle 111\rangle$

fcc $\lambda\{111\} \equiv \sigma_{cl.}\{111\}/G\{111\}\langle 112\rangle$

(Phys. Rev. B 91 (2015) 224203)



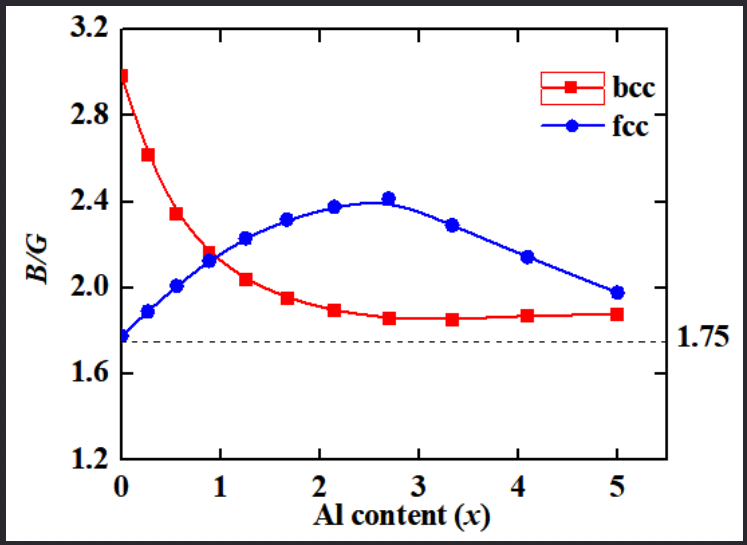
η=(λ(*x*)-λ(0))/λ(0)



Cauchy pressure $CP=C_{12}-C_{44}$

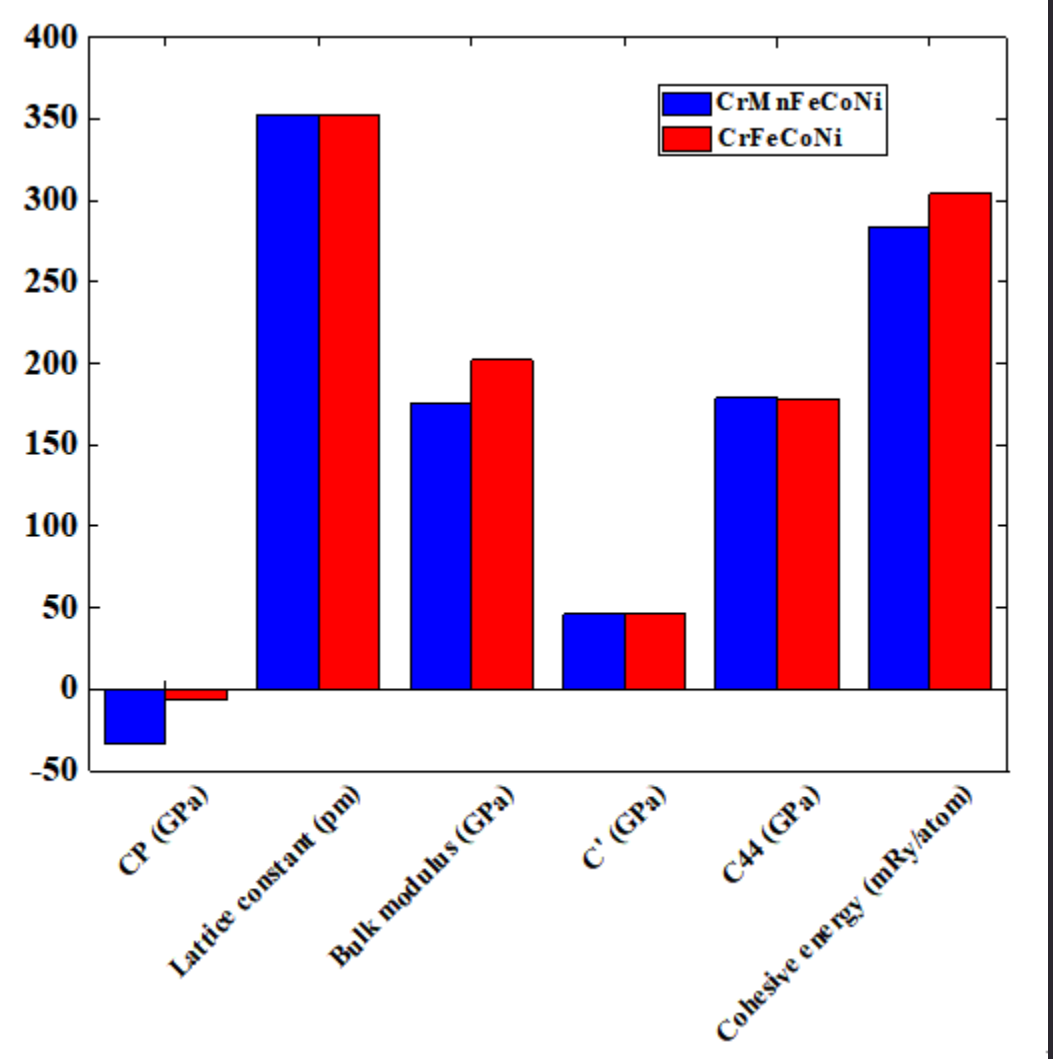
Ductile

Brittle



Pugh ratio *B/G*

Discussion



$CP \equiv B\text{-}C_{44}\text{-}2/3\ C'$

CrMnFeCoNi

CrFeCoNi

Summary

Using *ab initio* calculations, we provide the elastic constants of paramagnetic $Al_xCrMnFeCoNi$ ($0 \leq x \leq 5$) high-entropy alloys (HEAs) in both body-centered cubic (bcc) and face-centered cubic (fcc) structures

The brittle/ductile transitions formulated in terms of Cauchy pressure and Pugh ratio become consistent only when the strong elastic anisotropy is accounted for.

The negative Cauchy pressure of CrMnFeCoNi is due to the relatively low bulk modulus and C_{12} elastic constant, which in turn are consistent with the relatively low cohesive energy.

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Thanks for your attention !

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