Introduction to Solid Solution Strengthening with *GreenALM*

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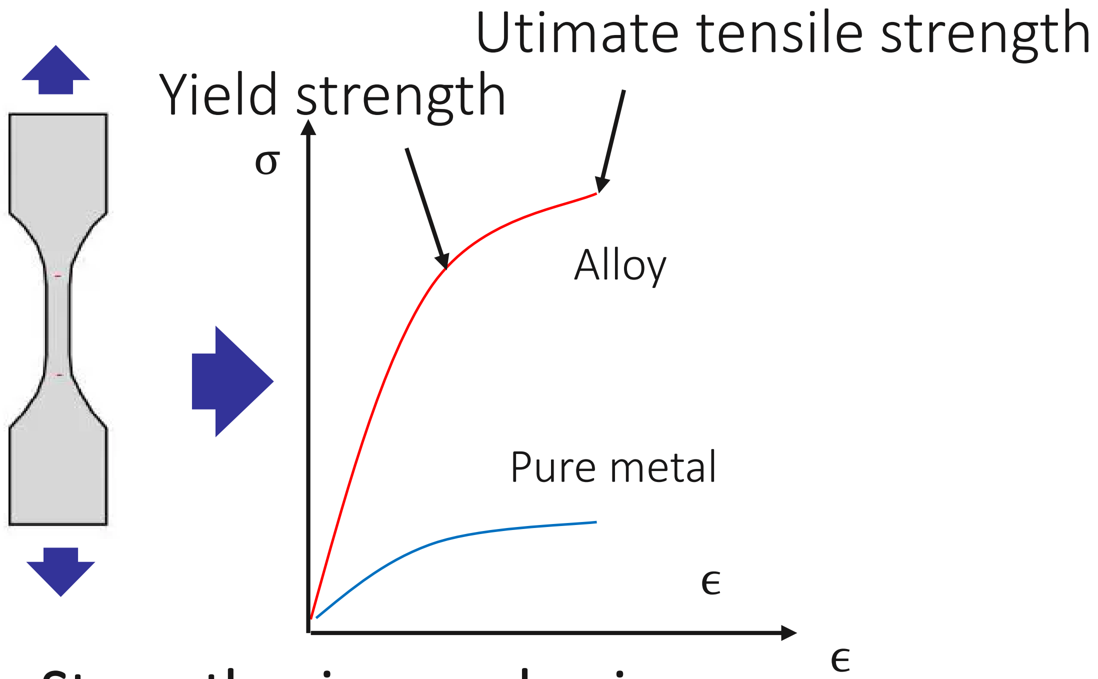
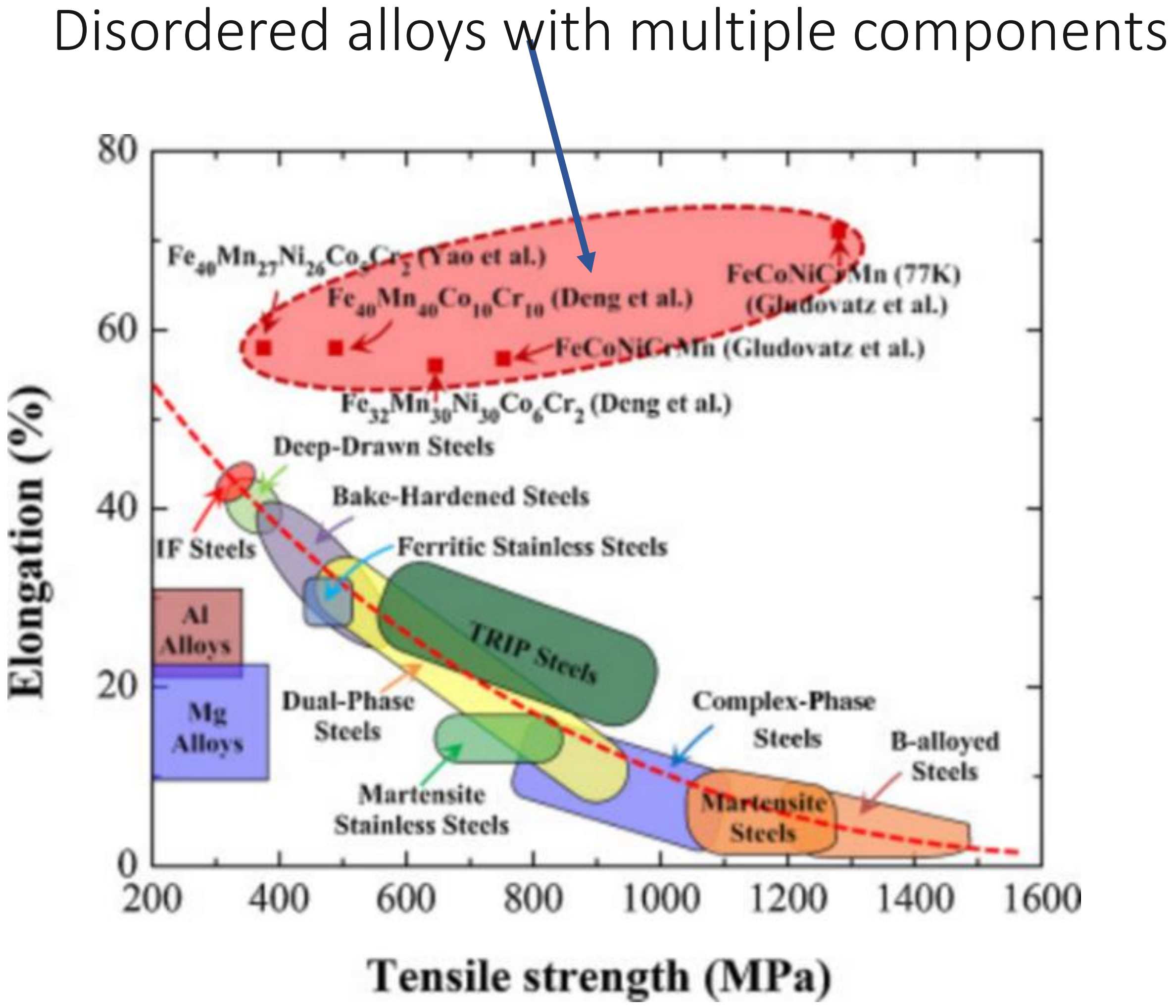
GreenALM Tutorials, 14.10.2021

We asked 100 People how they define strength





Strengthening mechanisms

- Grain boundary strengthening
- Precipitation strengthening
- Work hardening
- Transformation strengthening
- Solid solution Strengthening

Y. Yifan, *Materials Today* (2015)

Disordered alloys with multiple components

- Overcome ***strength-ductility trade off:*** Ductility due to cubic phase + significant solute solution strengthening

Difficulties in modelling solute-dislocation interaction

- Explicit calculation is out of reach for ab-initio
- Model approach: strength only using bulk materials properties. Conventional supercell approach too demanding.

Possible solution

- Green‘s function DFT methods for calculating substitutionally and magnetically disordered alloys.

Experimentally validated model for strength only using bulk materials properties of the alloy

$$\Delta\tau = f\left(C_{44}, C', B, \frac{\partial V_{Alloy}}{\partial c_i}; T\right)$$

Linear elastic parameters (for C_{44}, C', B)

Volume misfit of solute and matrix (for $\frac{\partial V_{Alloy}}{\partial c_i}; T$)

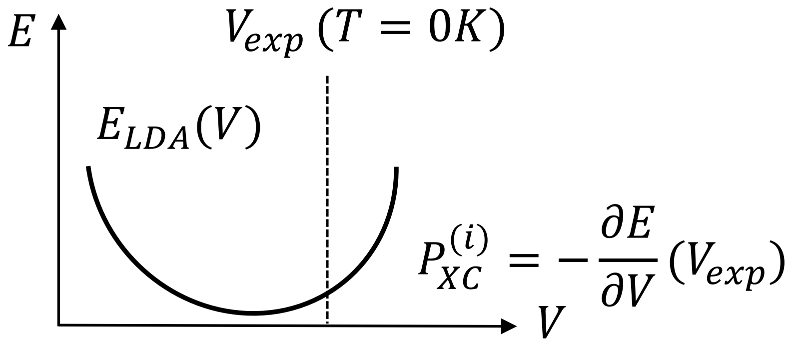
C. Varvenne, *Acta Materialia* **18**, 164 (2016)

Accurate prediction of the equilibrium volumes

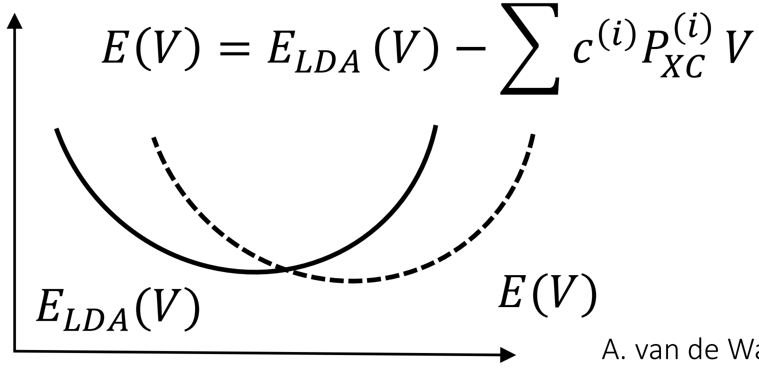
$\Delta\tau$:Critical resolved shear stress (CRSS)

Semiempircal correction of exchange-correlation effects

Element in ground state



Randomly disordered alloy

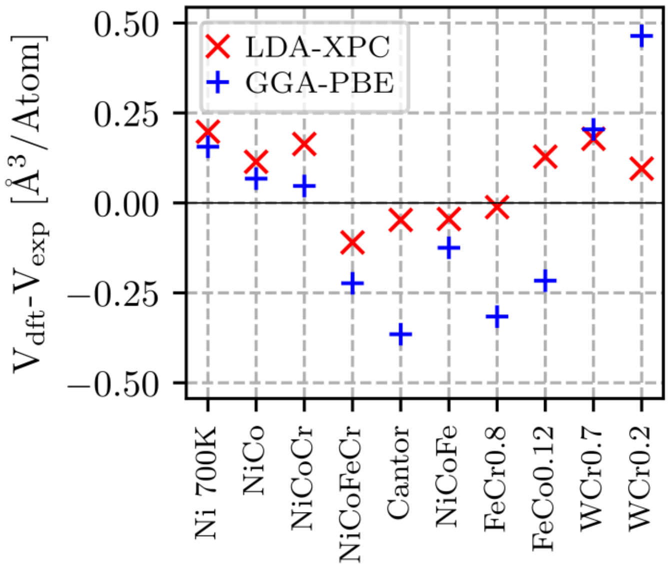


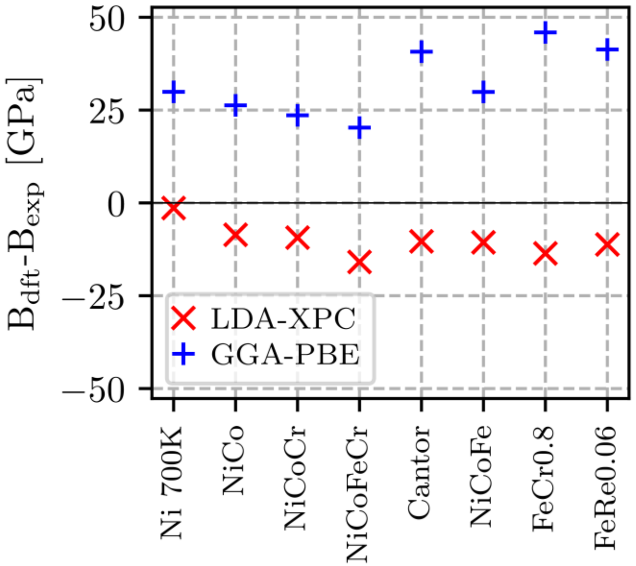
A. van de Walle and G. Ceder. *PRB* **59**, 14992 (1999)

Non-local exchange-correlations effects are included a-posteriori by an element specific pressure

Effects of pressure correction:

- Corrects systematic errors of the XC functional
- Improves prediction of linear response properties
- Transferable methodology





Input: Alloy $\{c^{(n)}, c^{(n+1)}, \dots, c^{(m)}\}$

$c^{(n)}$… concs. of element n in alloy [at. %]

Supercell Green‘s function DFT (LSGF)

CPA Green‘s function DFT

Finite temperature effects (phononic, magnetic, electronic)

C_{44}, C', B

$\frac{\partial V_{alloy}}{\partial c^{(n)}}$

Strengthening model

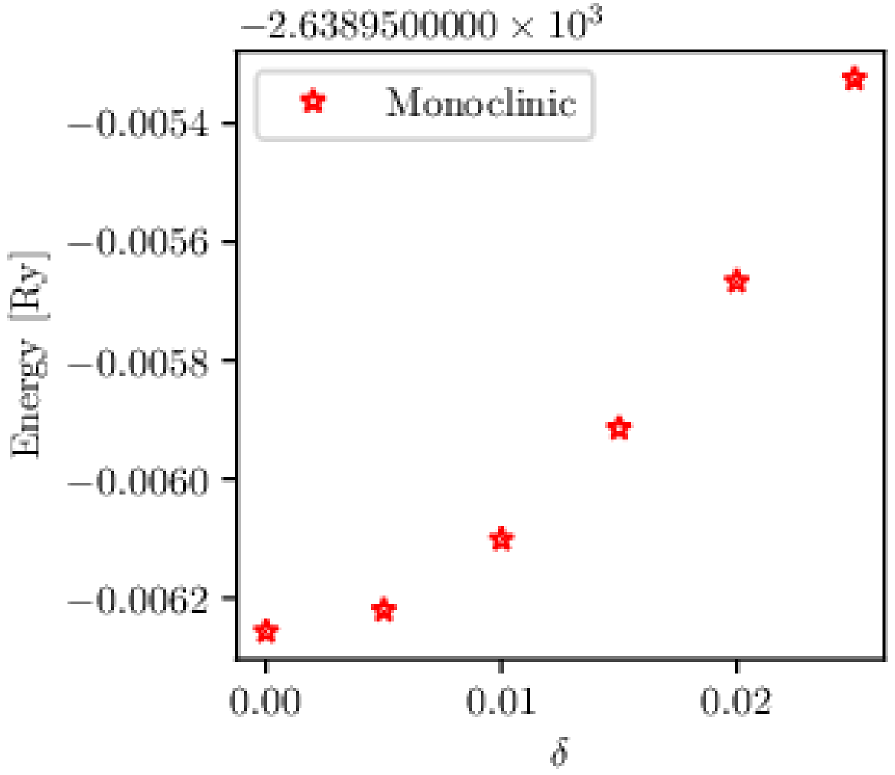
$\Delta\tau = f(C_{44}, C', B, \frac{\partial V_{Alloy}}{\partial c_i}; T)$

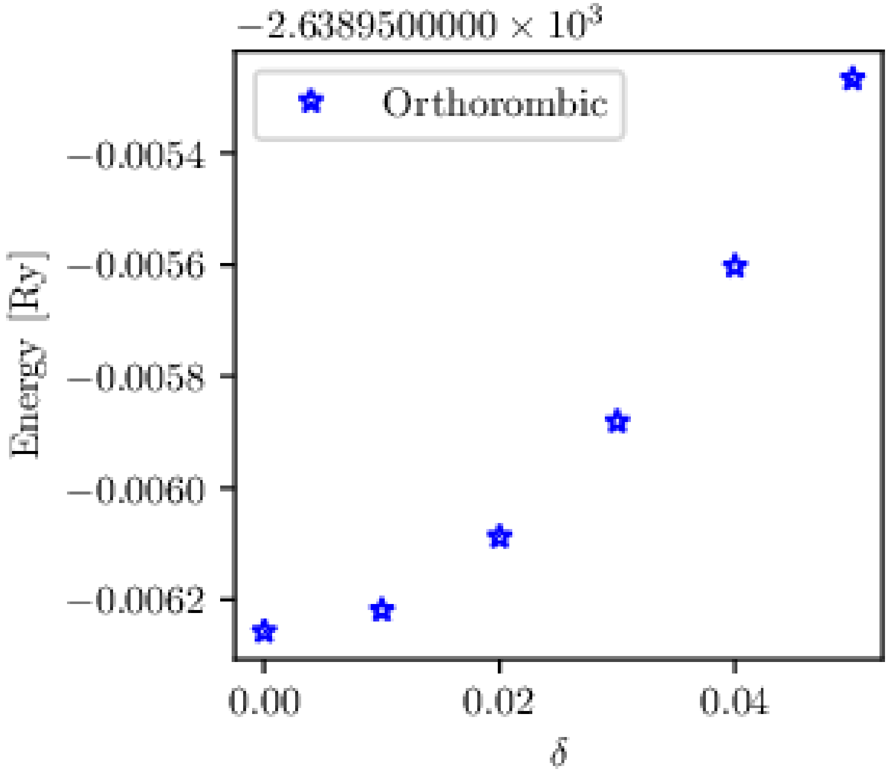
C. Varvenne, *Acta Materialia* **18**, 164 (2016)

Target quantity: $\Delta\tau_0$ Critical resolved shear stress

Workflow gives the critical resolved shear stress (CRSS) contribution due to solute solution strengthening

Volume conserving orthorombic and monoclinic distortions → C' C_{44}





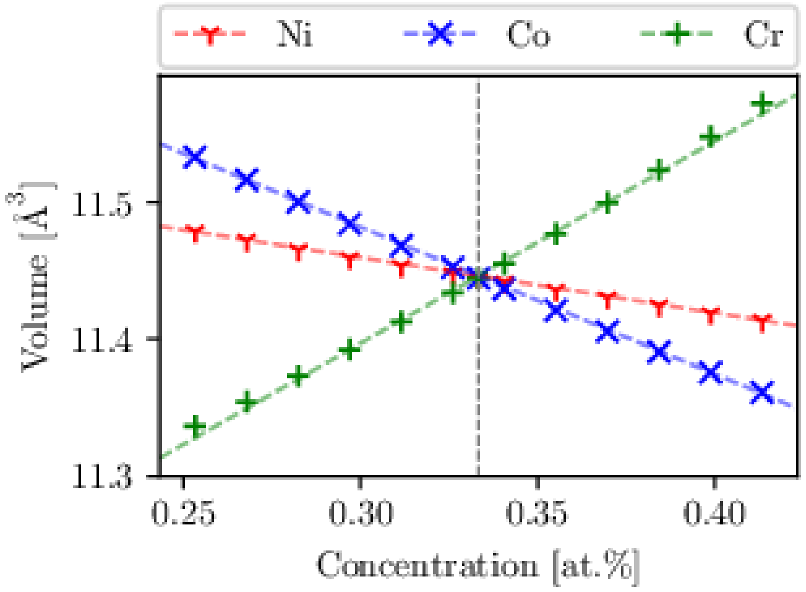
- Concentration constrain: simple finite difference won't work

$$\frac{\partial V_{alloy}}{\partial c^{(n)}} \qquad V_{alloy} = V_{alloy}(\{c_i\}) \qquad 1 = \sum c_i$$

- Fit to a linear function that takes into account constrain

$$V_{alloy} = a_0 + \sum_{i=1}^{n} a_i c_i$$

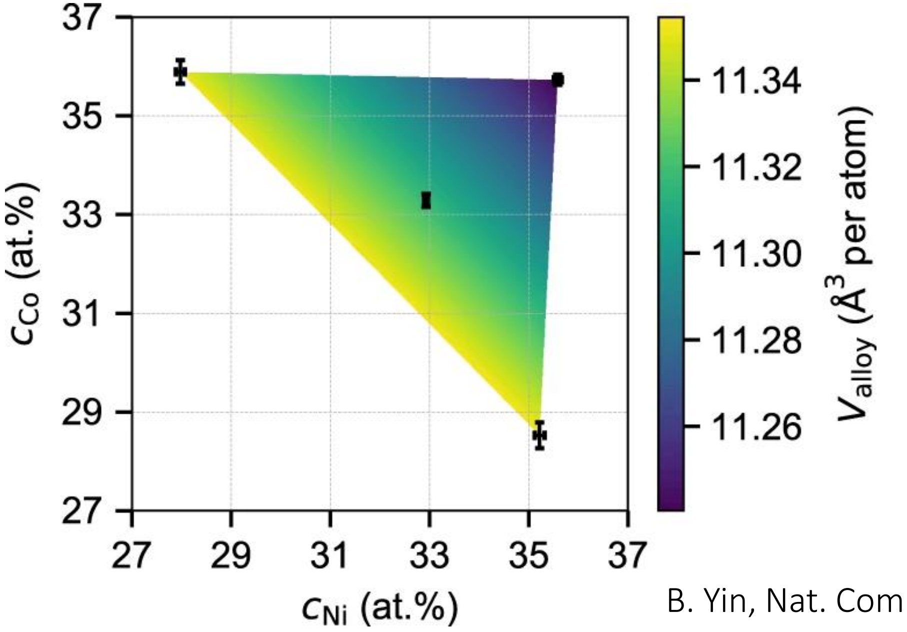
Concentration dependency is linear



Validation of input quantities for the strengthening in NiCoCr

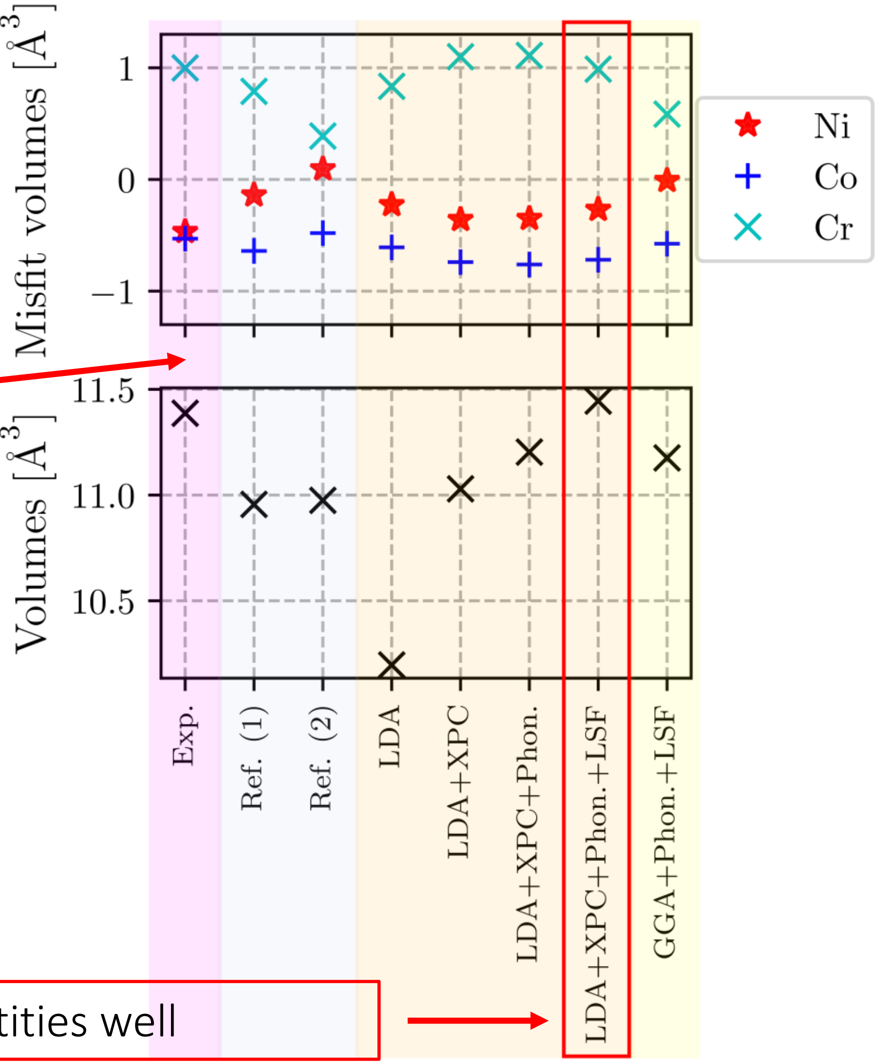
NiCoCr is rare example for **directly** measured misfit volumes

Misfit volume from finite difference approach:



B. Yin, Nat. Comm. (2020)

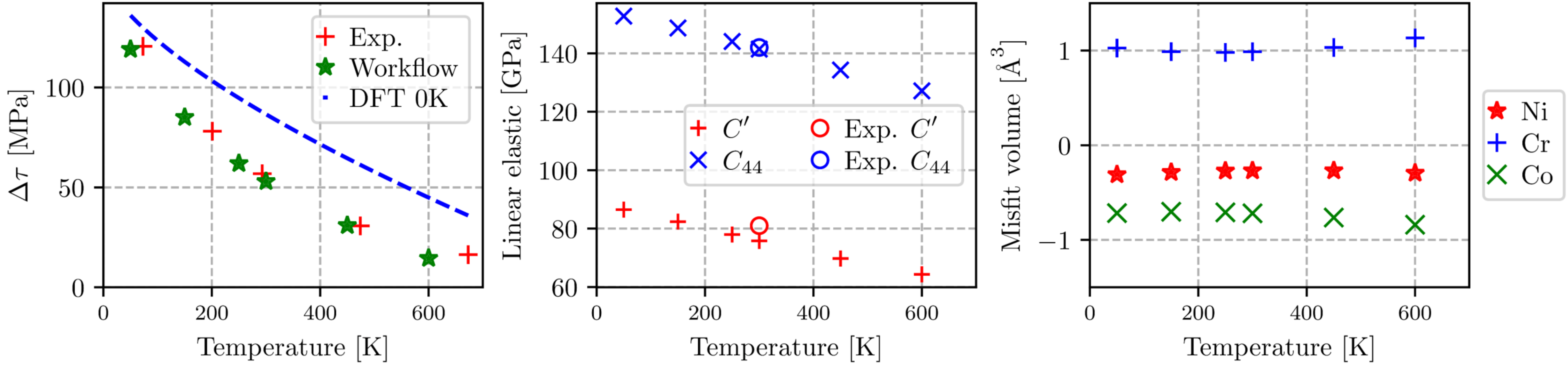
$$\frac{\partial V_{alloy}}{\partial c^{(n)}}$$



Full model predicts both quantities well

Prediction of temperature dependency of SSS in NiCoCr

Comparison strength from experiment[1] and ab-initio workflow



Exp.: [1] Z. Wu, *Acta Materialia* (2014)

Exp.: [2] H. Bei, *Materials Sci. a. Eng. A* (2017)

Sources of temperature dependency of $\Delta\tau$:

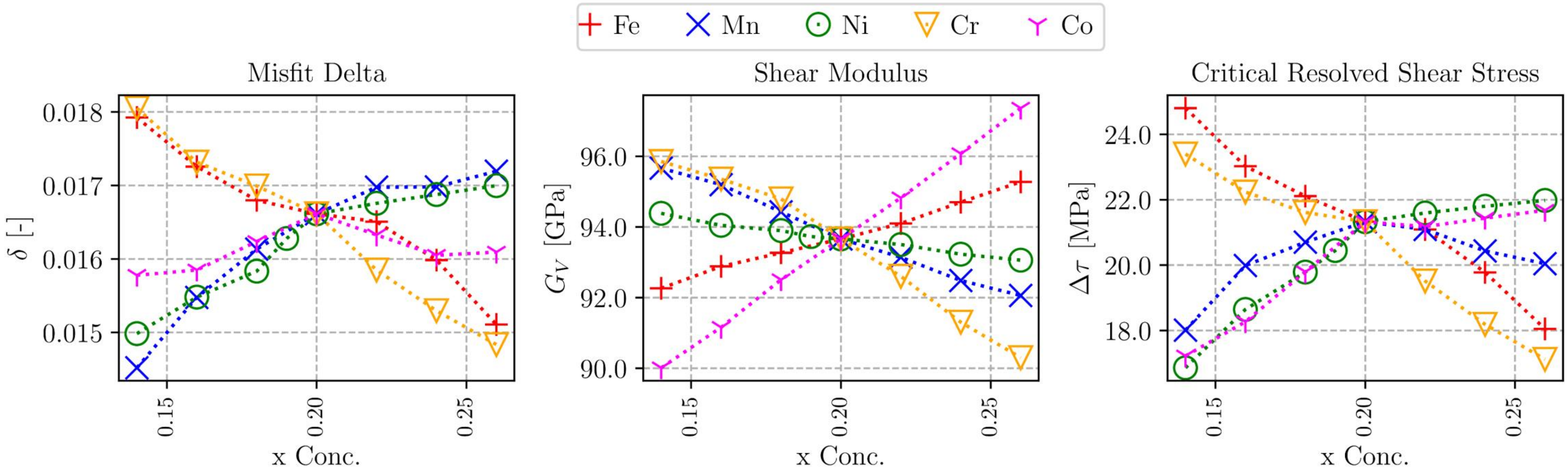
- Arrhenius-like dependency due to thermal activation mechanism
- Linear elastic constants and misfit volumes

Energy barrier is also temperature-dependent

Influence of concentration changes on the strength

Screening of FeMnNiCoCr (Cantor) alloy

Changing concentration of one component while ratio amongst the others are kept constant: e.g. $\{ Fe_x Mn_y Ni_y Co_y Cr_y \,|x + 4y = 1\}$



$\Delta\tau$ is mostly influenced by:

- Misfit delta δ: concentration-weighted RMS of misfit volumes
- Shear modulus G_V

Result suggest that a reduced Fe or Cr is beneficial for the strength