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Computational Mechanical and Materials Engineering

Multi-scale simulation of mechanical properties and solid solution strengthening

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Virtual Psi-k GreenALM Hands-on Tutorial 2021 – MCL Leoben (Austria)

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Multiscale Mechanics Modelling

a brief overview

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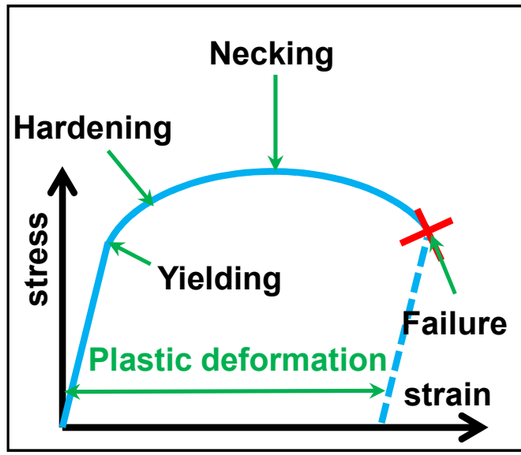
Materials: multi-scale and complex

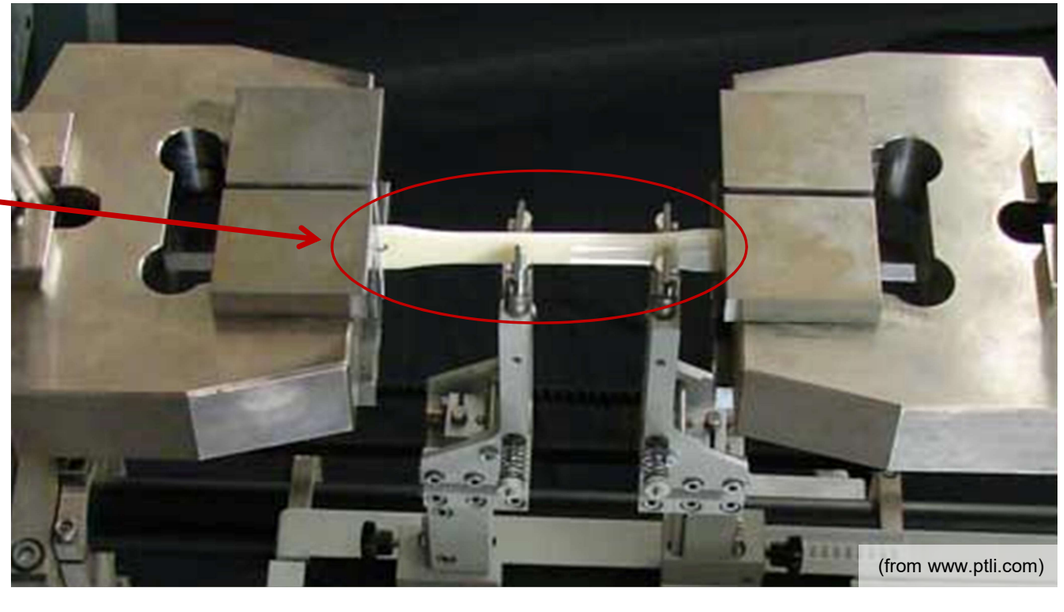
Challenges for *understanding* and *modelling*:

1. **Intrinsically multi-scale**
2. **All scales important (in general)**
3. **Complexity gives *emergent* macroscopic properties**



Component scale (cm to m)

tensile test



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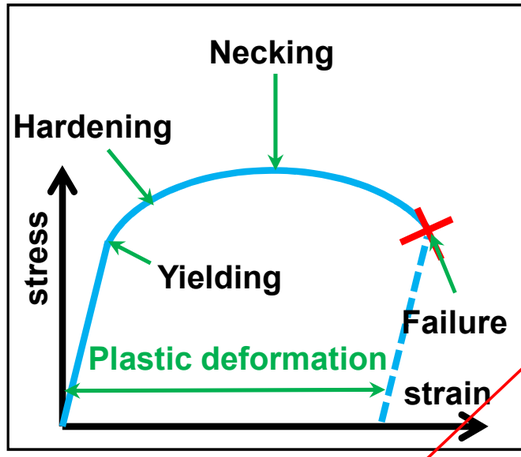
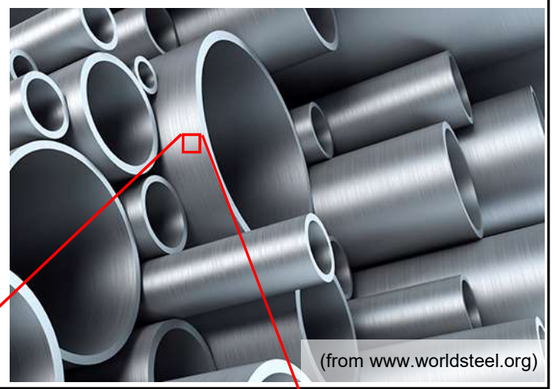
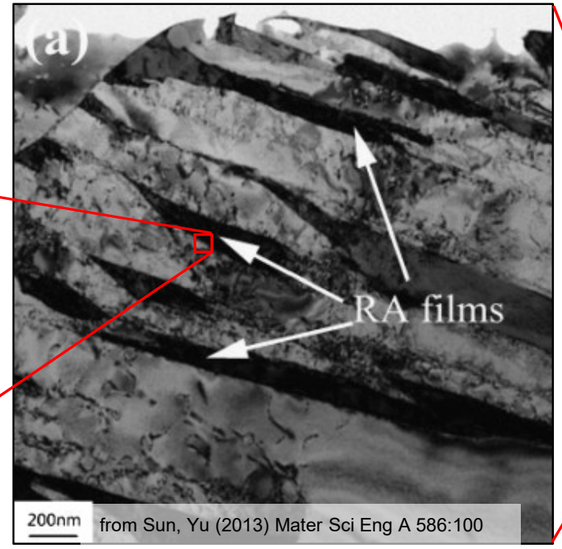


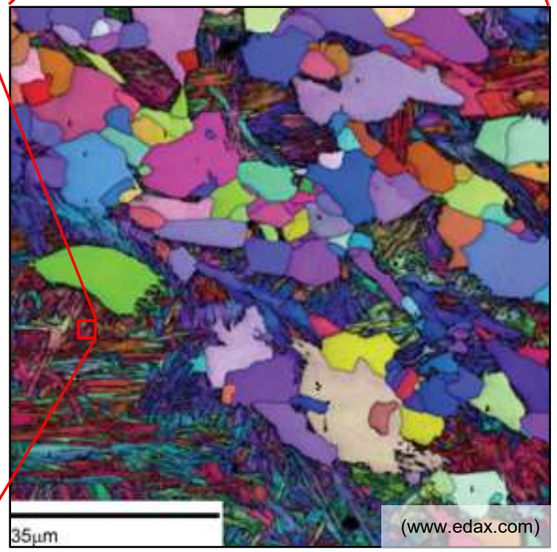
Component scale (cm to m)



Nano-/Micro-scale (nm to μm)

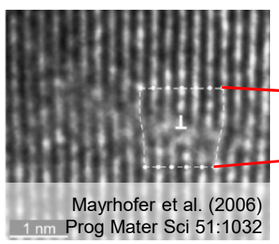


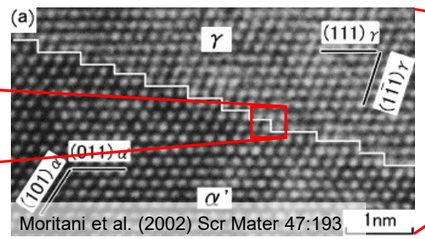
Mesoscale (μm to mm)



Nano- and Microstructures

Atomistic/Nanoscale
(Å to few nm)



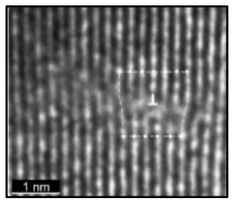


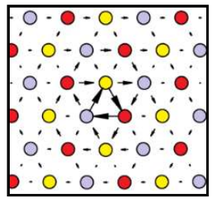
Dislocations **Interfaces**

Multi-scale modelling

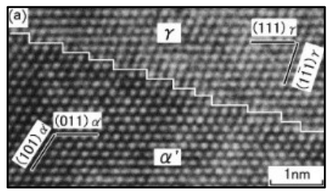
$time$

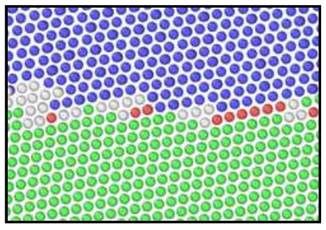
Complexity: coupled, nonlinear phenomena occur at different length- and time-scales



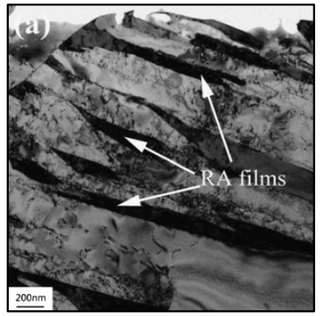


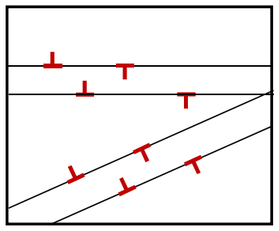
Quantum Mechanics



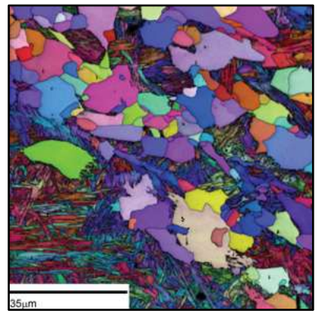


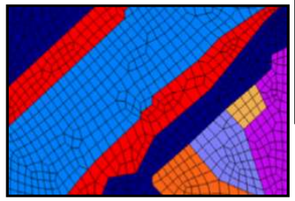
Molecular Dynamics



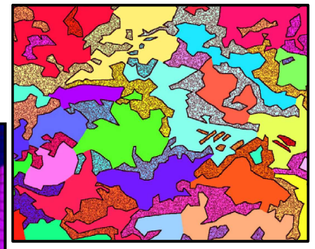


Discrete Dislocations

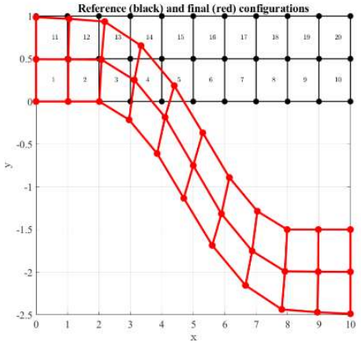




Crystal Plasticity



Micromechanics



Macroscale modelling

Atomistics

$10^{-10}\ m$ $10^{-9}\ m$ $10^{-6}\ m$ $10^{-3}\ m$ $1\ m$

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Solid solution strengthening

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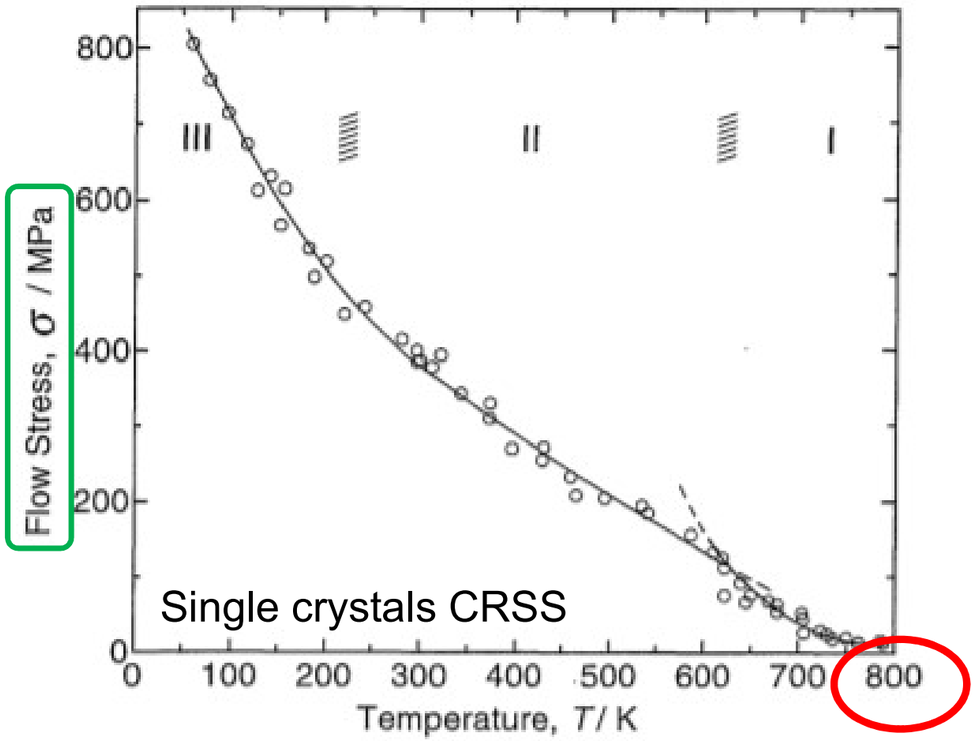
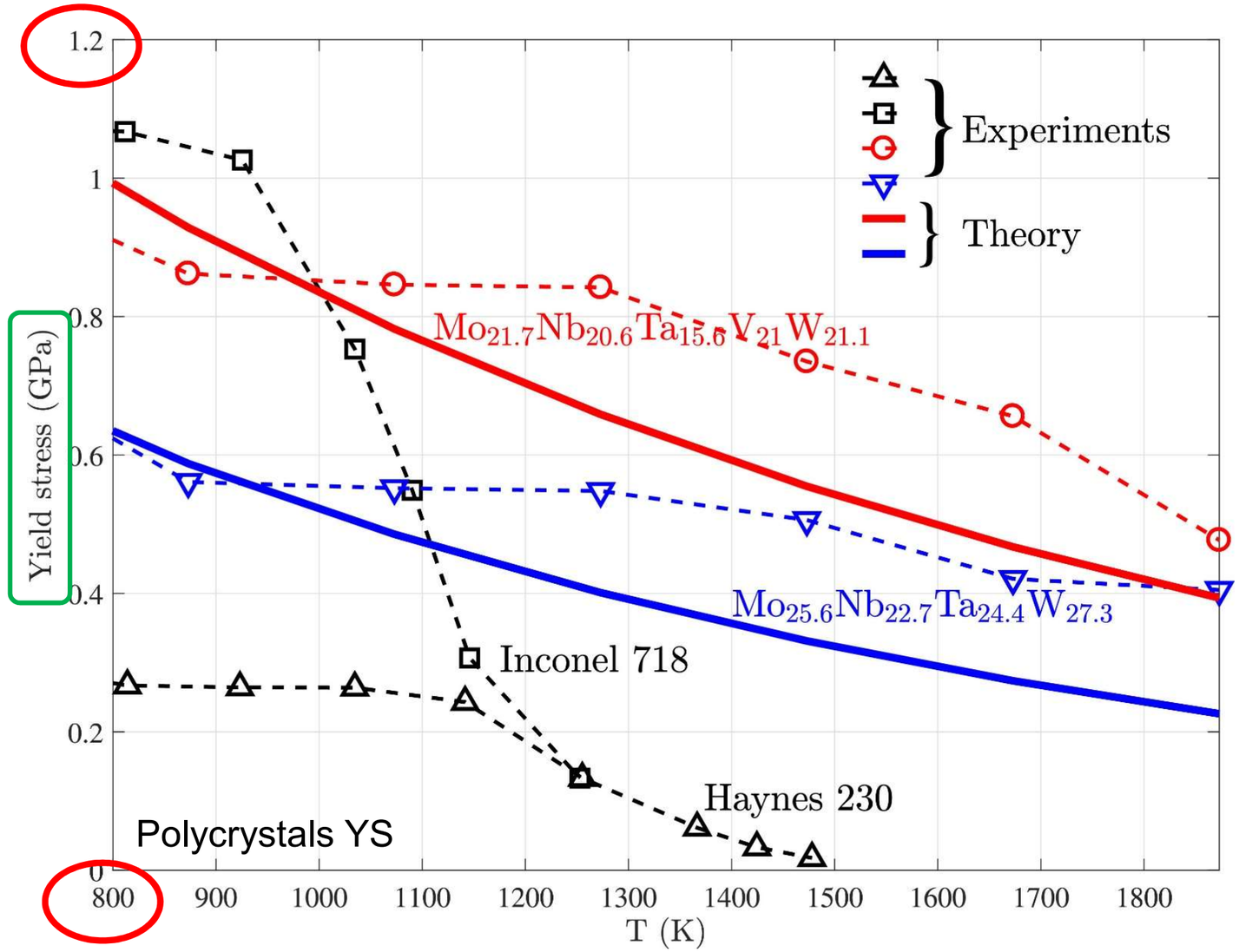
Solid solution strengthening in random alloys

Motivation 1: Large strengthening observed compared with elemental metals. **Why?**

Brunner (2000) Mater Trans JIM 41, 152





Solid solution strengthening – F. Maresca (U. Groningen)

Senkov, Wilks, Scott, Miracle (2011) Intermetallics 19, 698
Maresca, Curtin (2020) Acta Mater 182, 235

Solid solution strengthening in random alloys

Motivation 2: Immense compositional space, trial-and-error unfeasible. **Predictive model?**

High Entropy Alloys (HEAs)
[Multi Principal Element Alloys, MPEAs]
[Complex Concentrated Alloys, CCAs]

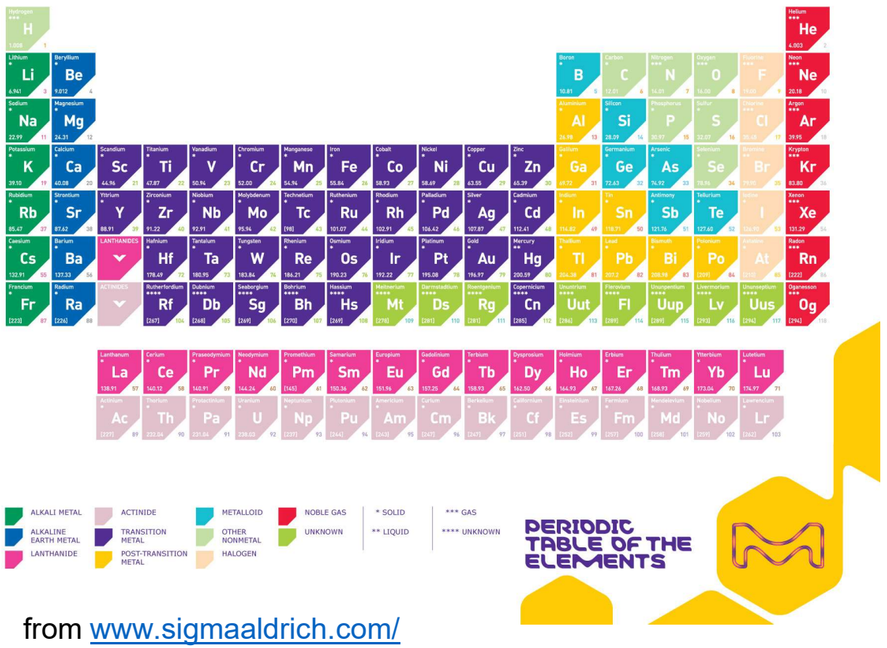
Senkov, Miracle (2017) Acta Mater 122, 448

Yeh et al. (2004) Adv Eng Mater 6, 299

Solid solutions favored by config. entropy over brittle intermetallics

$\Delta S_{\mathrm{conf}} \sim R \ln N$ R gas constant, N: # of elements

[Neglects formation enthalpy, other entropy contributions]



from www.sigmaaldrich.com/

$\mathcal{O}(40)$ metals (no toxic/radioactive/rare)

→ $\sim 10^{78}$ combinations (Cantor 2014 Entropy 16, 4749)

>> Avogadro's number! $(6.022 \cdot 10^{23})$

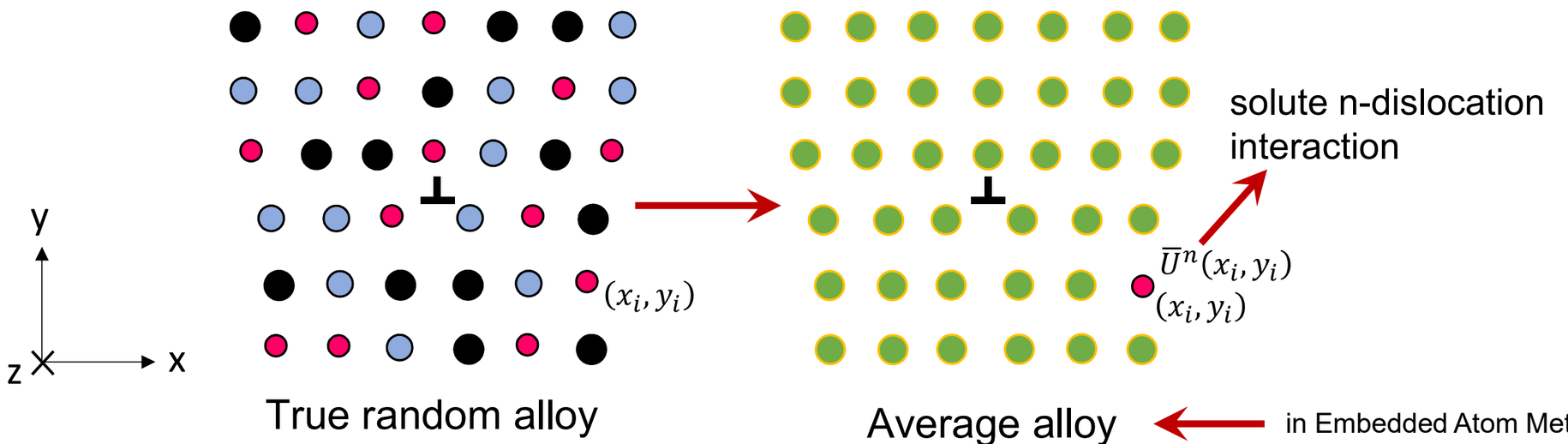
Theory of strengthening in random alloys

N component alloy

***Recent review of solute strengthening theories:**
Varvenne, Leyson, Ghazisaeidi, Curtin (2017) Acta Mater 124, 660

c_n concentration of the *n-th* element $\left(\sum_{n=1,N} c_n = 1\right)$

Dislocation exists in homogeneous, “average” alloy



in Embedded Atom Method (EAM) context:
Varvenne, Luque, Nöhring, Curtin (2016) PRB 93, 104201

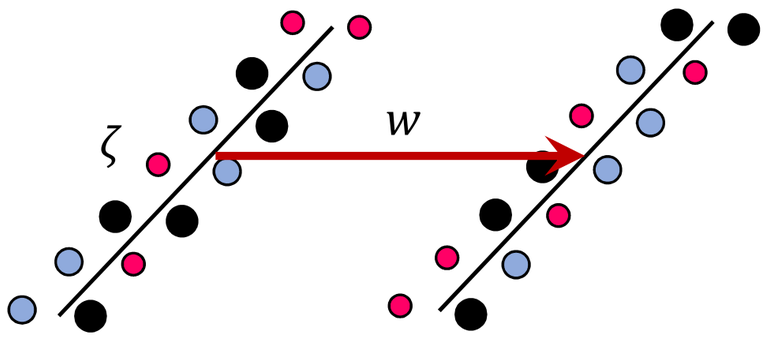
Average alloy effective matrix with **average properties** of true random alloy, e.g.:

1. lattice parameter
2. elastic constants
3. generalized stacking fault energy

Leyson, Hector, Curtin (2012) Acta Mater 60, 3873
Varvenne, Luque, Curtin (2016) Acta Mater 118, 164

Theory of strengthening in random alloys

$\Delta U_{tot}(\zeta, w)$ total energy change of dislocation segment ζ gliding by w



$\Delta U_{tot}(\zeta, w)$ random variable* (zero avg.)

$$\sigma_{\Delta U_{tot}(\zeta,w)} = [\langle \Delta U_{tot}^2(\zeta, w)\rangle - \langle \Delta U_{tot}(\zeta, w)\rangle^2]^{\frac{1}{2}}$$

$$= \left(\frac{\zeta}{\bar{\alpha} b}\right)^{\frac{1}{2}} \Delta \tilde{E}_p(w)$$

$\bar{\alpha}$ crystal and dislocation character specific

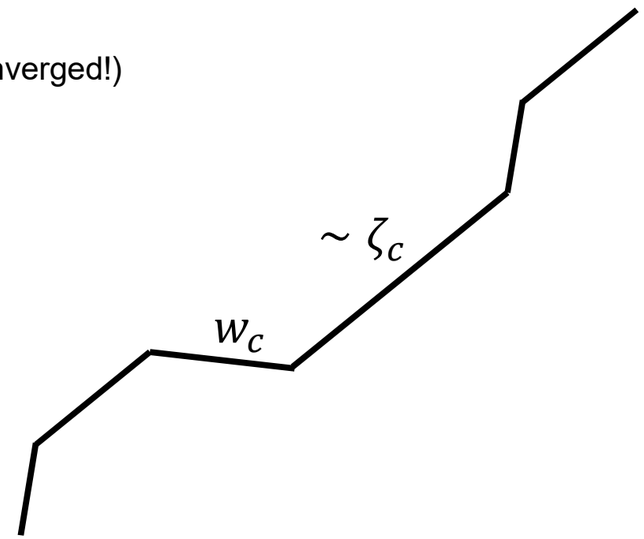
Key energy parameter for strengthening:

$$\Delta \tilde{E}_p(w) = \left[\sum_{\substack{i,j \\ n}} c_n \left(\bar{U}^n(x_i - w, y_j) - \bar{U}^n(x_i, y_j)\right)^2\right]^{\frac{1}{2}}$$

(infinite sum but converged!)

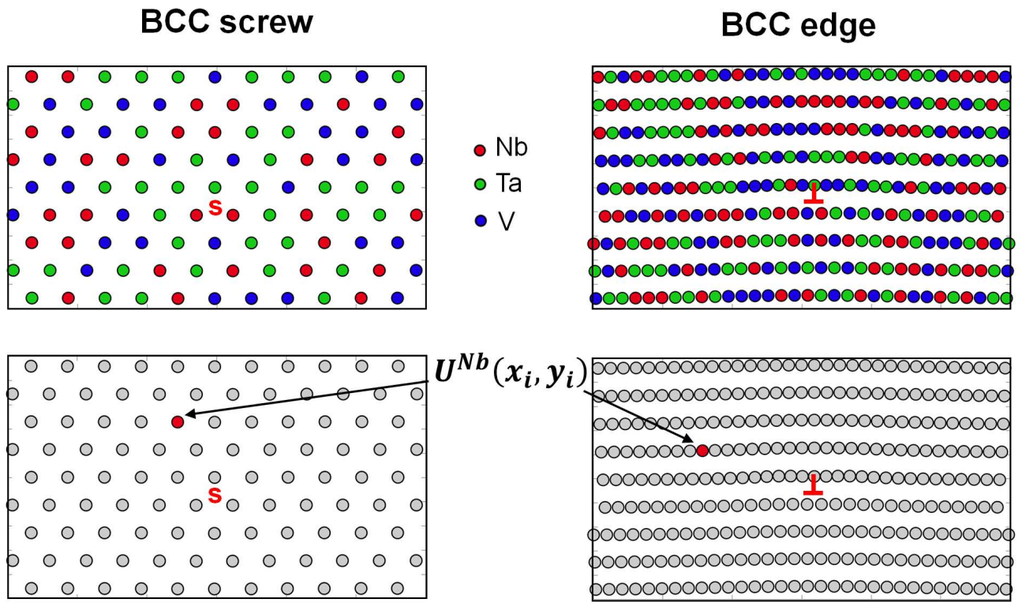
Dislocation attracted to low energy solute fluctuations and repelled by high energy solute fluctuations

→ Wavy dislocation structure $w_c, \sim \zeta_c$



Varvenne, Luque, Curtin (2016) Acta Mater 118, 164

Theory of strengthening in random alloys



Maresca and Curtin (2020) Acta Mater 182, 144
Maresca and Curtin (2020) Acta Mater 182, 235

True random alloy

Interaction energy in average atom matrix

Interaction energy map

$\bar{U}^n(x_i, y_i)$

Energy change after dislocation glides

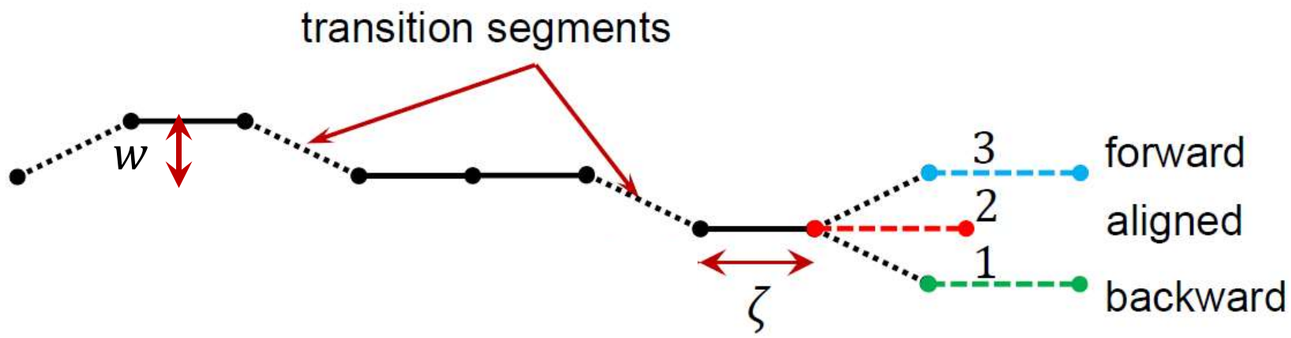
$\bar{U}^n(x_i - w, y_j) - \bar{U}^n(x_i, y_j)$

Theory of strengthening in random alloys

Minimum energy structure of dislocation of length L:

Maresca and Curtin (2020) Acta Mater 182, 144
Maresca and Curtin (2020) Acta Mater 182, 235

"three-choice" model



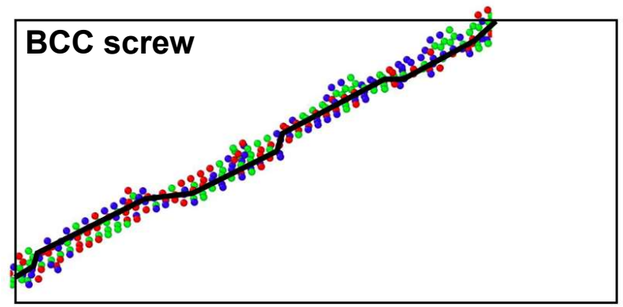
Total energy change w.r.t. straight dislocation: $\Delta \mathrm{E}^{tot} = E_L^{tot} - E_P^{tot}$

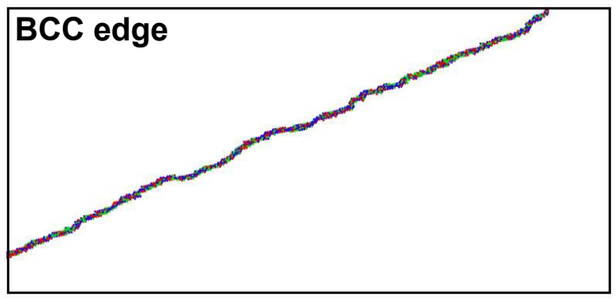
E_L^{tot}: contribution of joining segments (kinks, for BCC screws)

E_P^{tot}: contribution of ζ segments lowering the energy

ζ_c and w_c such that $\Delta \mathrm{E}^{tot}/L$ is minimum!

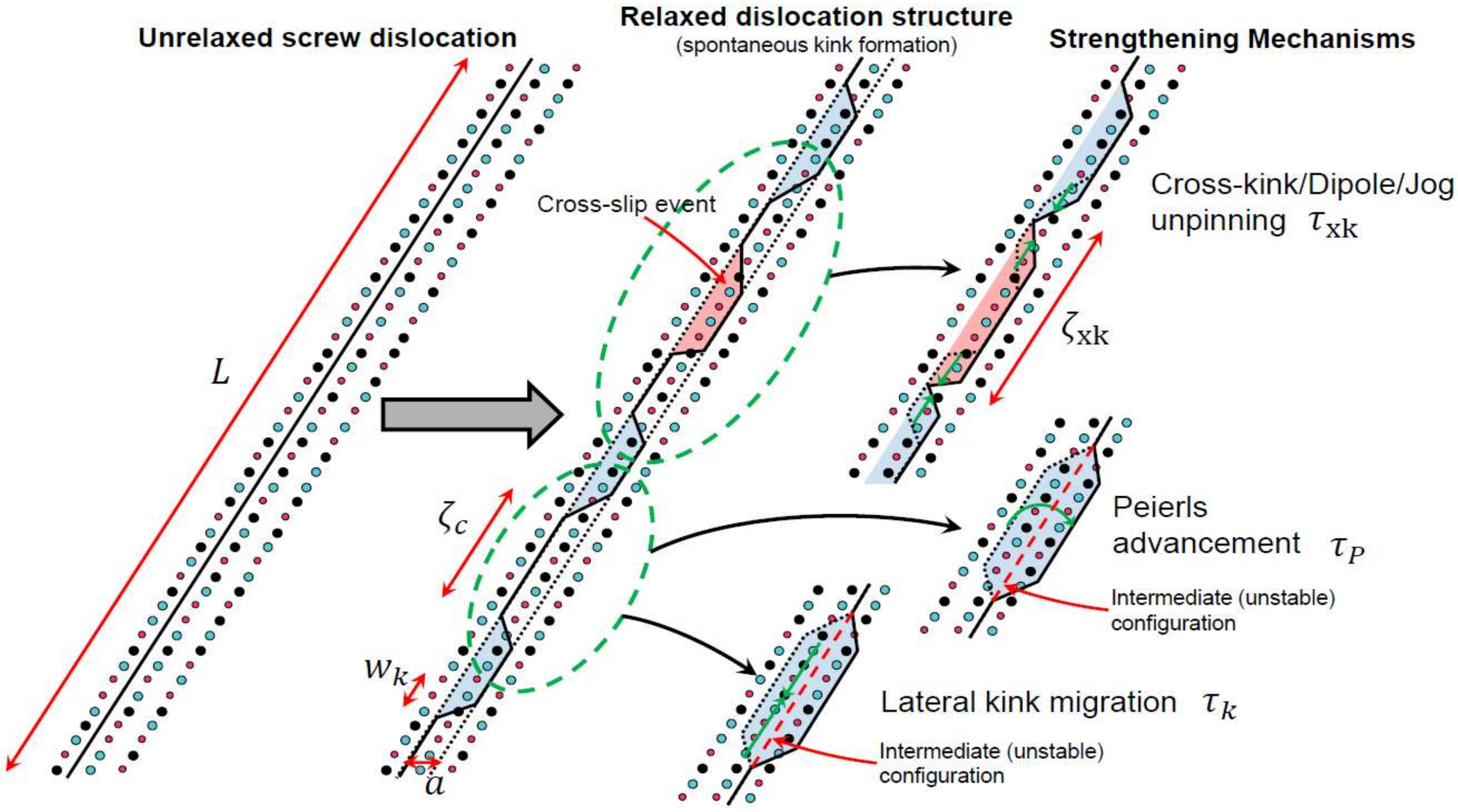
Energy barrier and T=0K CRSS and (→ finite T, rate-dependent behaviour) determined by minimum energy structure and energy scale parameter $\Delta \tilde{E}_p$





Varvenne, Luque, Curtin (2016) Acta Mater 118, 164

Theory of strengthening: Screw dislocations in BCC alloys



Maresca and Curtin (2020) Acta Mater 182, 144

Theory of strengthening: Screw dislocations in BCC alloys

$$\Delta \mathrm{E}^{tot}(\zeta, w)\ /L = \left[\kappa E_k - \beta \left(\frac{\zeta}{b}\right)^{\frac{1}{2}} \Delta\tilde{E}_p(w)\right] \frac{1}{(1+\kappa)\zeta}$$

E_L E_P

Total energy change per total length L

E_k kink energy

Length $w = a$ (Peierls valleys spacing), too costly to form longer kinks.

Minimizing w.r.t. ζ yields the penalization $E_L = \frac{1}{2} E_P$.

Then, $\kappa = 0.39$ and $\beta = 0.72$ are determined self-consistently (numerically)

Repeating unit: $2.5\ \zeta_c$ $w_c = a$

Characteristic **length scale**:

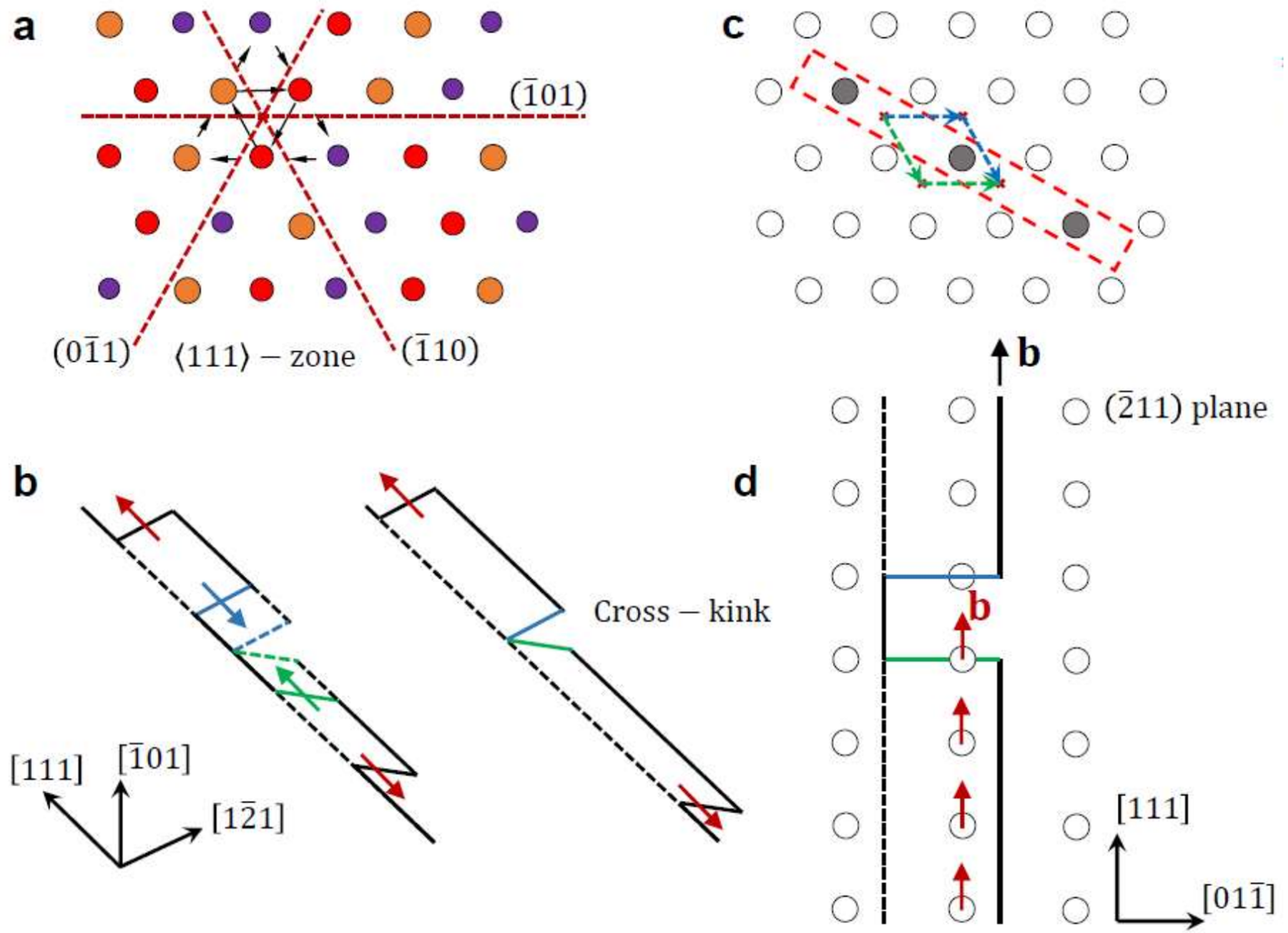
→ $\zeta_c = \left(1.083 \frac{E_k}{\Delta\tilde{E}_p}\right)^2$

Characteristic **energy barrier** in front of $2.5\ \zeta_c$ segments:

→ $\Delta E_b = 2.7\ E_k$ (also computed with three-choice model)

Theory of strengthening: Screw dislocations in BCC alloys

Cross-kink spacing: $\zeta_{xk} = 7.5\zeta_c$ ($\zeta_{xk} = 10\zeta_c$ for {112} slip)



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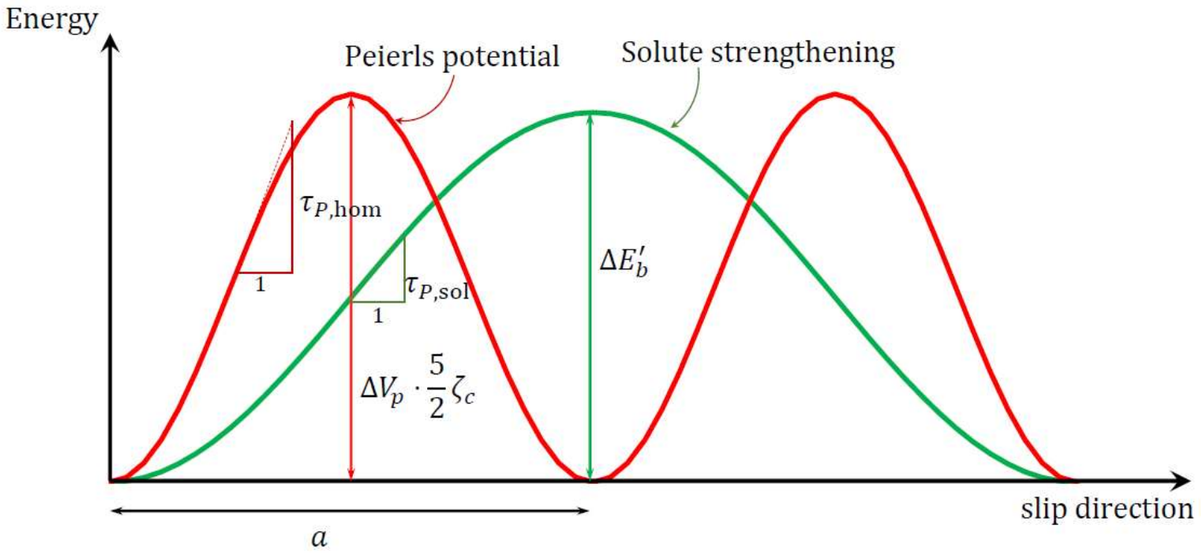
Theory of strengthening: Screw dislocations in BCC alloys

Strengthening mechanisms: Peierls mechanism (low T)

$\Delta E'_b = 2.7\ E_k - 2E_k = 0.7E_k$ (2 kinks are annihilated as a 2.5ζ_c segment moves forward)



Total enthalpy:

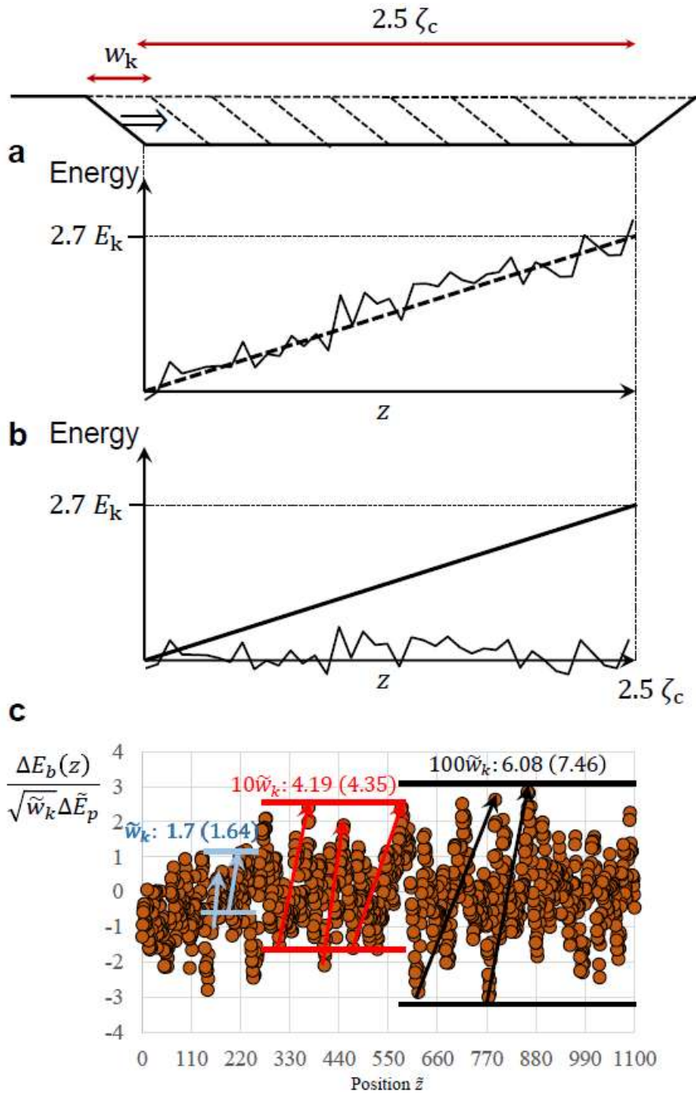
$$H_P(x) = \frac{\Delta E'_b}{2}\left[1 - \cos\left(\frac{\pi x}{a}\right)\right] + \frac{2.5\zeta_c \Delta V_P}{2}\left[1 - \cos\left(\frac{2\pi x}{a}\right)\right] - \frac{5}{2}\tau b \zeta_c x$$

Total enthalpy barrier:

$$\rightarrow \quad \Delta H_P(\tau) = \Delta E_{b,P}\left(1 - \frac{\tau}{\tau_{P,0}}\right)^{\frac{3}{2}}$$

Theory of strengthening: Screw dislocations in BCC alloys

Strengthening mechanisms: Kink glide mechanism (intermediate T)



Total enthalpy:

$$H_{\mathrm{k}}(z) = 1.37\sqrt{w_{\mathrm{k}}/b}\Delta\tilde{E}_p \ln\left(2.3\frac{z}{w_{\mathrm{k}}}+1\right) + 1.37E_{\mathrm{k}}\frac{z}{2.5\zeta_c} - \frac{\tau abz}{2}$$

Total enthalpy barrier:

$$\Delta H_{\mathrm{k}}(\tilde{\tau}_{\mathrm{k}}) = 1.37\sqrt{w_{\mathrm{k}}/b}\Delta\tilde{E}_p\left(\tilde{\tau}_{\mathrm{k}} - \ln\tilde{\tau}_{\mathrm{k}} - 1\right)$$

$$\tilde{\tau}_{\mathrm{k}} = \frac{\tau-\tau_b}{\tau_{\mathrm{k},0}-\tau_b}$$

Stress vs enthalpy:

$$\frac{\tau-\tau_b}{\tau_{\mathrm{k},0}-\tau_b} = \left[\exp\left(0.89\Delta\tilde{H}_{\mathrm{k}} + 0.5\Delta\tilde{H}_{\mathrm{k}}^{\frac{1}{4}} + 0.6\right) - 1\right]^{-1}$$

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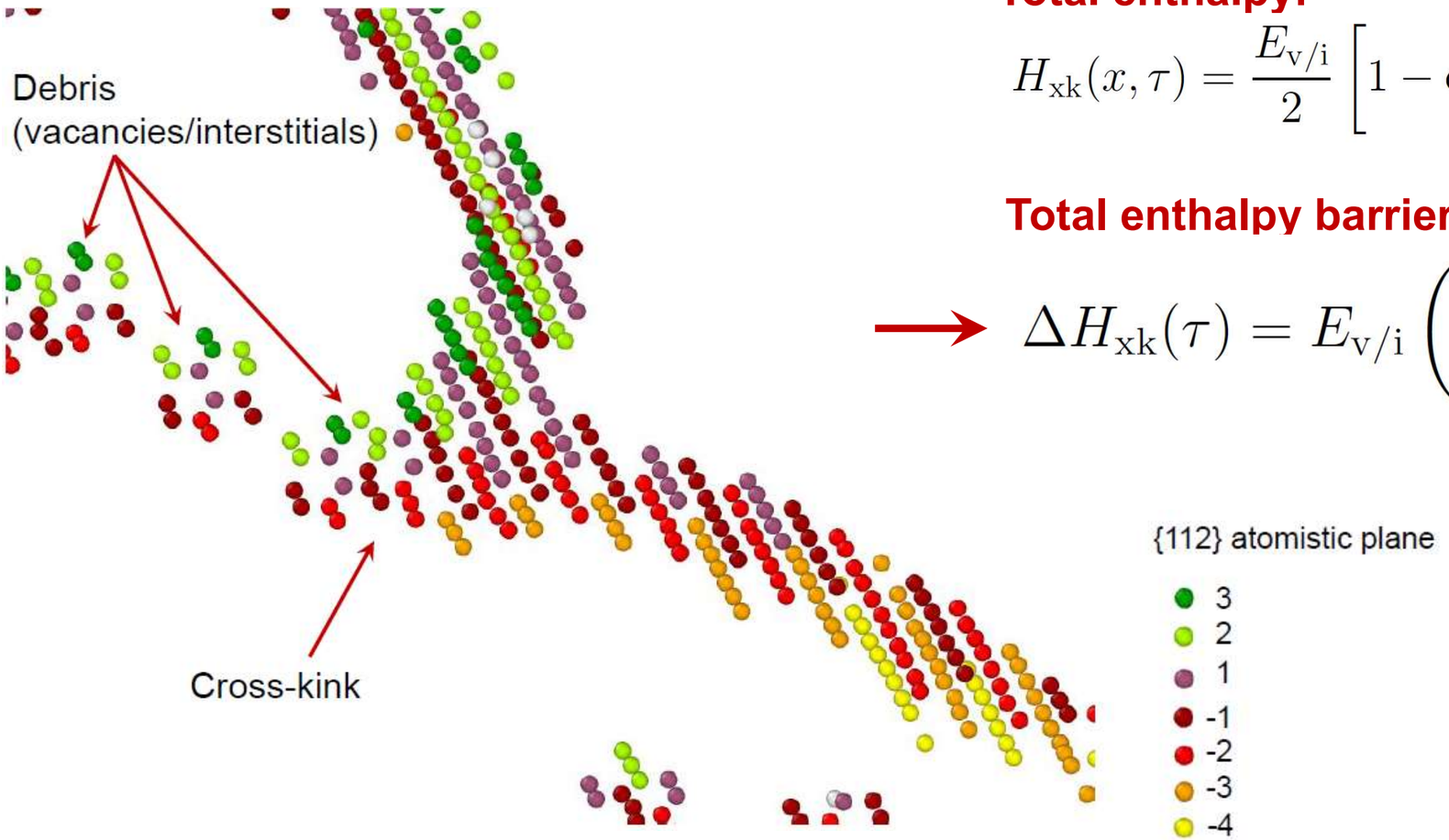
Theory of strengthening: Screw dislocations in BCC alloys

Strengthening mechanisms: Cross-kink mechanism (moderate to high T)

Standard analysis for creation of point defects:



Total enthalpy:

$$H_{\mathrm{xk}}(x,\tau) = \frac{E_{\mathrm{v/i}}}{2}\left[1-\cos\left(\frac{2\pi x}{a}\right)\right] - \tau b x \zeta_{\mathrm{v/i}}$$

Total enthalpy barrier:

$$\rightarrow \Delta H_{\mathrm{xk}}(\tau) = E_{\mathrm{v/i}}\left(1-\frac{\tau}{\tau_{\mathrm{xk},0}}\right)^{\frac{3}{2}}$$

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Theory of strengthening: Screw dislocations in BCC alloys

Screw dislocations strengthening mechanisms: analytical theory

$$\tau(\dot{\varepsilon},T) = \tau_{\mathrm{xk}}\left(\dot{\varepsilon},T\right) + \min\left[\tau_{\mathrm{k}}\left(\dot{\varepsilon},T\right), \tau_P\left(\dot{\varepsilon},T\right)\right]$$

where

$$\tau_{\mathrm{xk}}\left(\dot{\varepsilon},T\right) = \tau_{\mathrm{xk},0}\left[1-\left(\frac{\Delta H}{E_{\mathrm{v/i}}}\right)^{\frac{2}{3}}\right]$$

Cross-kinking

$$\tau_{\mathrm{k}}\left(\dot{\varepsilon},T\right) = \tau_b + \frac{\tau_{\mathrm{k},0}-\tau_b}{\left\{\exp\left[0.89\frac{\Delta H}{\Delta E_{\mathrm{k},0}} + 0.5\left(\frac{\Delta H}{\Delta E_{\mathrm{k},0}}\right)^{\frac{1}{4}} + 0.6\right] - 1\right\}}\ , \quad \frac{\tau-\tau_b}{\tau_{\mathrm{k},0}-\tau_b} > \frac{1}{3.45\frac{\zeta_c}{w_{\mathrm{k}}}+1}\ ,$$

$$\tau_{\mathrm{k}}\left(\dot{\varepsilon},T\right) = \tau_b - (\tau_{\mathrm{k},0}-\tau_b)\frac{w_{\mathrm{k}}}{3.45\zeta_c}\frac{\Delta H}{\Delta E_{\mathrm{k},0}}\ , \quad \frac{\tau-\tau_b}{\tau_{\mathrm{k},0}-\tau_b} < \frac{1}{3.45\frac{\zeta_c}{w_{\mathrm{k}}}+1}\ ,$$

Kink glide

$$\tau_P(\dot{\varepsilon},T) = \tau_{P,0}\left[1-\left(\frac{\Delta H}{\Delta E_{b,P}}\right)^{\frac{2}{3}}\right]\ .$$

Peierls mechanism

Finite temperature/strain rate behaviour by using an Arrhenius model, $\Delta H = kT\ln\left(\frac{\dot{\varepsilon}_0}{\dot{\varepsilon}}\right)$

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Theory of strengthening: Screw dislocations in BCC alloys

All theory quantities expressed w.r.t. few material parameters:

1) Kink energy E_k

2) Solute-dislocation interaction parameter $\Delta\tilde{E}_p$

3) Vacancy/self-interstitial formation energies $E_{\mathrm{v/i}}$

4) Peierls barrier ΔV_P

$$\zeta_c = \left(1.083\frac{E_\mathrm{k}}{\Delta\tilde{E}_p}\right)^2 b$$

$$\tau_{\mathrm{xk},0} = \frac{\pi E_{\mathrm{v/i}}}{ab\zeta_{\mathrm{v/i}}} \qquad (\zeta_\mathrm{v} = 7.5\zeta_c,\ \zeta_\mathrm{i} = 15\zeta_c)$$

$$\tau_b = \frac{1.08E_\mathrm{k}}{ab\zeta_c}$$

$$\tau_{\mathrm{k},0} = \frac{6.3\Delta\tilde{E}_p}{ab^2\sqrt{w_\mathrm{k}/b}} + \tau_b$$

$$\Delta E_{\mathrm{k},0} = 1.37\sqrt{w_\mathrm{k}/b}\Delta\tilde{E}_p$$

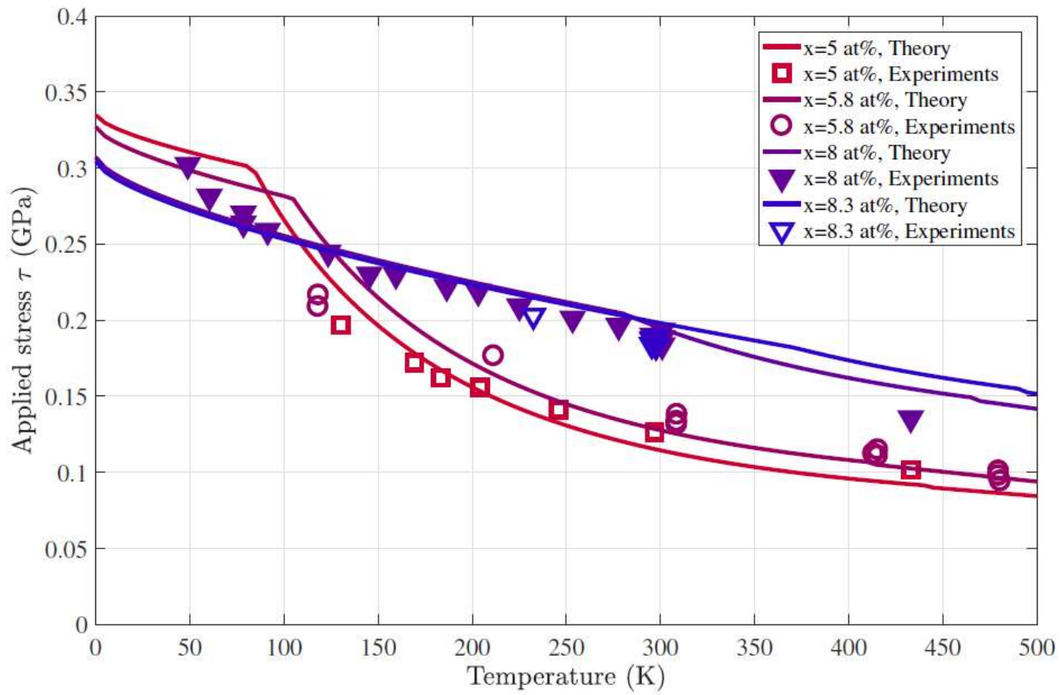
$$\tau_{P,0} = \frac{\pi\Delta V_P}{ba} + \frac{0.44E_\mathrm{k}}{ba\zeta_c}\left[1 - \frac{5\Delta V_P\zeta_c}{(20\Delta V_P\zeta_c + 0.7E_\mathrm{k})}\right]$$

$$\Delta E_{b,P} = \frac{(10\Delta V_P\zeta_c + 0.7E_\mathrm{k})^3}{(20\Delta V_P\zeta_c + 0.7E_\mathrm{k})^2}\ .$$

Maresca and Curtin (2020) Acta Mater 182, 144

Theory of strengthening: Screw dislocations in BCC alloys

Theory vs Fe-Si alloys



X-kink spacing in Fe 9%Si:
185 nm
(expts Caillard: 143 +/-54 nm)

Theory predictions for $Fe_{1-x}Si_x$ alloys.

Input:

Alloy	a_0 (Å)	$\Delta\tilde{E}_p$ (meV)	E_k (eV)	E_v (eV)	E_{si} (eV)	$\Delta\tilde{V}_P$ (meV)
$Fe_{95}Si_5$	2.864	39.8	0.4932	2.22	5.1	6.6
$Fe_{94.2}Si_{5.8}$	2.864	43.0	0.4932	2.22	5.1	5.9
$Fe_{92}Si_8$	2.861	50.5	0.4932	2.22	5.1	3.9
$Fe_{91.7}Si_{8.3}$	2.861	51.4	0.4932	2.22	5.1	3.7

Only 2 quantities fitted.

Expts.

Single fit, $\sqrt{c}$ scaling

Fe GAP

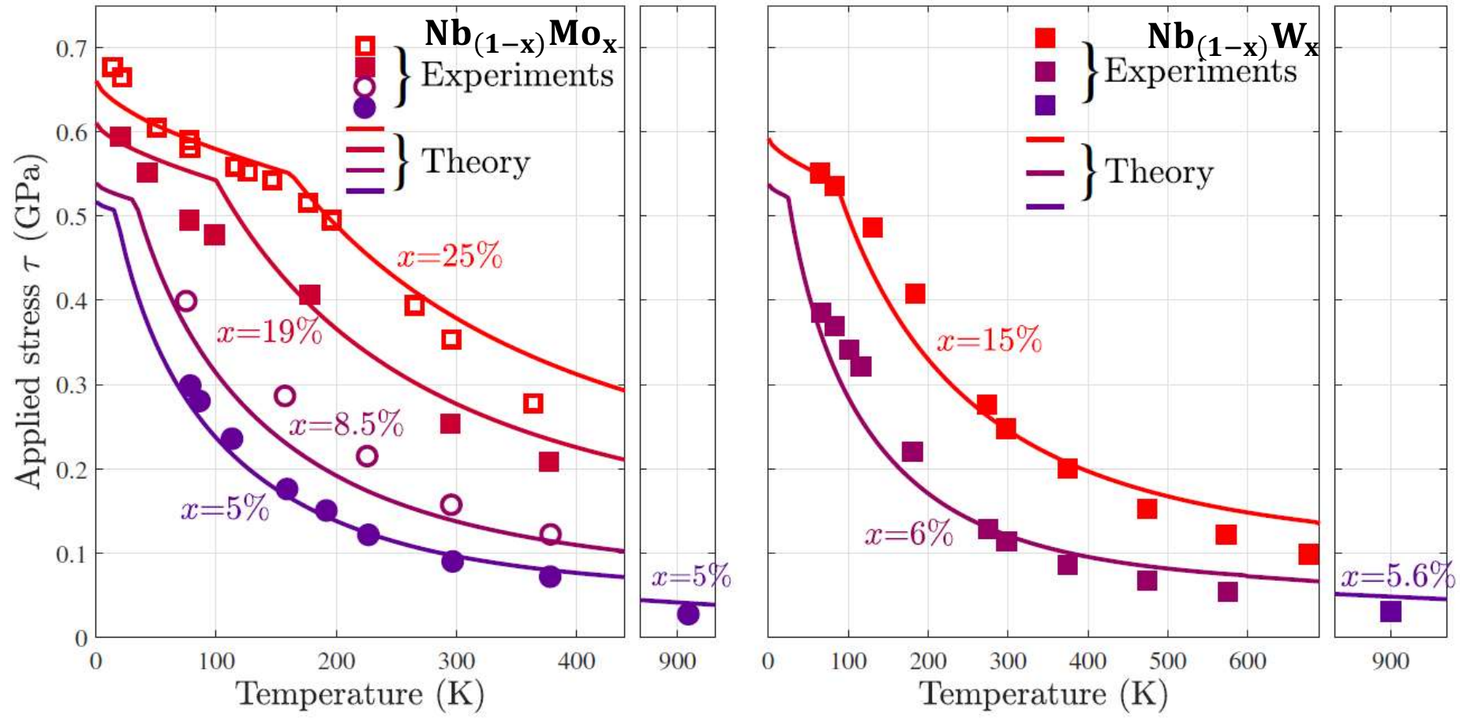
DFT

Standard solute softening, single fit

Maresca and Curtin (2020) Acta Mater 182, 144

Theory of strengthening: Screw dislocations in BCC alloys

Theory vs Nb-Mo and Nb-W



Input:

Alloy	a_0 (Å)	$\Delta\tilde{E}_p$ (meV)	E_k (eV)	E_v (eV)	E_{si} (eV)	$\Delta\tilde{V}_P$ (meV)
$Nb_{95}Mo_5$	3.289	48.8	0.6342	2.989	5.361	20
$Nb_{91.5}Mo_{8.5}$	3.282	56.2	0.6302	2.987	5.437	20
$Nb_{81}Mo_{19}$	3.261	74.5	0.6182	2.984	5.664	20
$Nb_{75}Mo_{25}$	3.250	84.7	0.6112	2.983	5.794	20
$Nb_{95.4}W_{5.6}$	3.290	52.4	0.6548	3.022	5.494	20.5
$Nb_{94}W_6$	3.289	54.1	0.6559	3.024	5.511	20.5
$Nb_{85}W_{15}$	3.275	73.2	0.6798	3.076	5.897	20.5

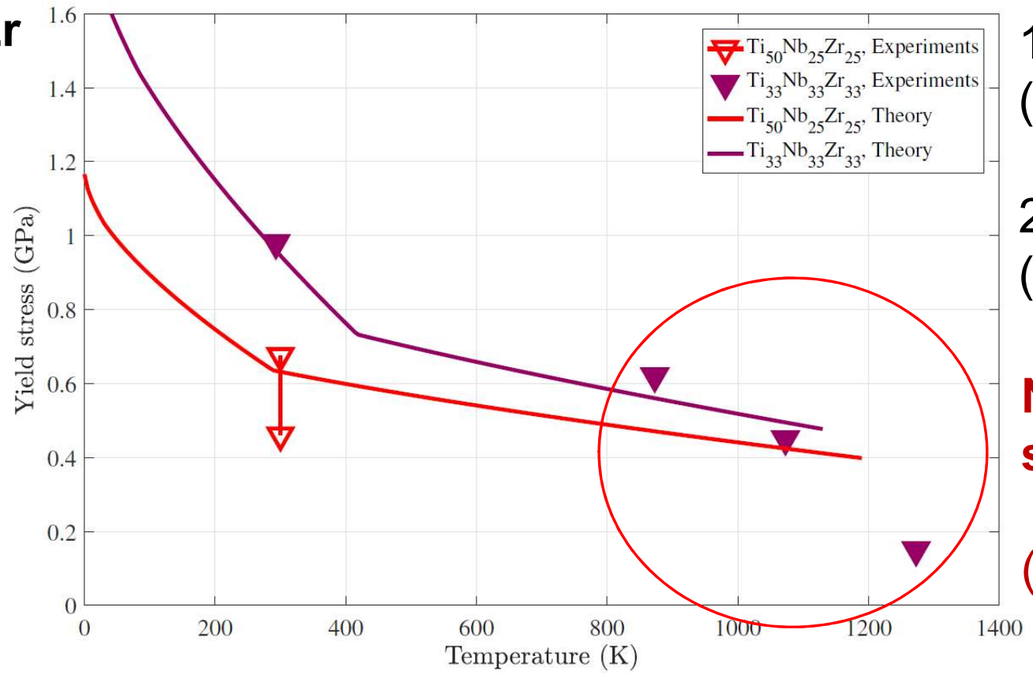
Expts. | Single fit, $\sqrt{c}$ scaling | DFT | single fit

Only 2 quantities fitted.

Maresca and Curtin (2020) Acta Mater 182, 144

Theory of strengthening: Screw dislocations in BCC alloys

Theory vs Nb-Ti-Zr



1) X-kink spacing Ti50Nb25Zr25: 42 nm (expts Mompiou et al.: 63 +/-30 nm)

2) ~RT $V_{act} = 48b^3$ and $57b^3$ (comparable to $48b^3$ in TiZrHfNbTa)

No high temperature strength!

(drop at ~ $T_m/2$)

Input:

Alloy	a_0 (Å)	$\Delta\tilde{E}_p$ (meV)	E_k (eV)	E_v (eV)	E_{si} (eV)	$\Delta\tilde{V}_P$ (meV)
$Ti_{33}Nb_{33}Zr_{33}$	3.393	71.0	0.255	1.868	3.535	10.7
$Ti_{50}Nb_{25}Zr_{25}$	3.365	63.5	0.256	1.745	3.404	4

Only 2 quantities fitted.

Expts.

MD, scaled by 1 common prefactor

MD

MD, scaled by 1 common prefactor

Theory of strengthening: Screw dislocations in BCC alloys

Conclusions – Screw theory

Fully derived parameter-free theory for screw dislocation strengthenig from dilute to “high entropy” alloys.

1) **Minimum energy screw dislocation kinked** in alloys: kink nucleation *not* the controlling mechanism

2) The theory is based on three **main mechanisms** (Peierls, kink glide and cross-kinking) acting at different temperature regimes, with **cross-kinking** dominant at higher T.

3) Theory **rationalizes** the main experimental results on Fe-Si, Nb-Mo, Nb-W alloys and on Nb-Ti-Zr HEAs

4) In screw-controlled Nb-Ti-Zr, **no high strength retention** above 1300K.

Challenges:

[e.g. notable WRe, WTa cases, Li, Draxl, Wurster, Pippan, Romaner (2017) PRB 95, 094114]

Theory input (especially $\Delta\tilde{E}_p$, but see also ΔV_P) cannot be determined yet *ab-initio*

An opportunity for exploration with CPA / GreenALM?

Theory of strengthening: Edge dislocations in BCC alloys

Motivations:

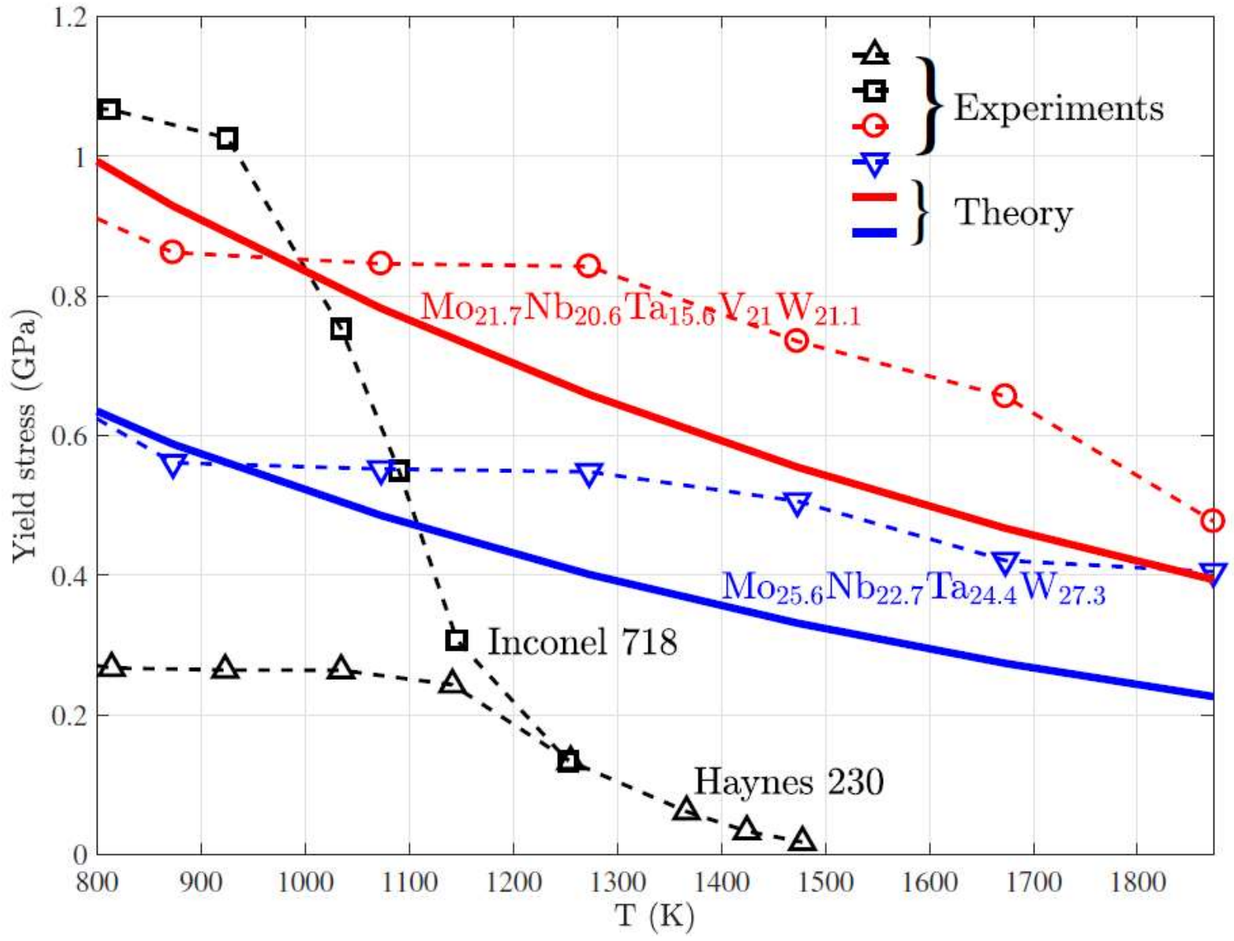
1. Screw-controlled Ti-Nb-Zr
   not retaining strength above 1300K:

   different mechanism responsible
   for high-T strength in MoNbTaVW?

2. Experiments in NbMo* and FeSi**
   reveal decreased edge mobility
   w.r.t. screws

3. X-ray line analysis in TiZrHfNbTa
   indicate edge dislocations
   dominance at yielding***

4. Yield strengths correlate with solute
   misfit volume (Yao et al. 2017) → hallmark of edge strengthening!

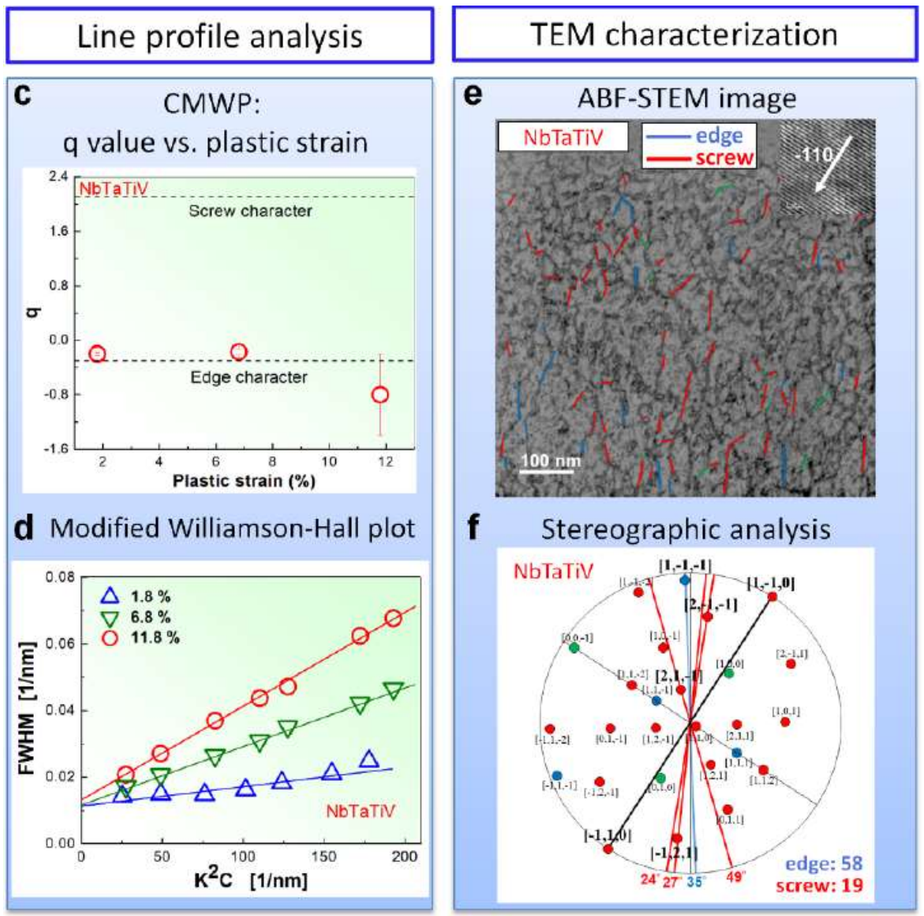


*Statham, Koss and Christian (1972); **Caillard (2013); ***Dirras et al. (2015)

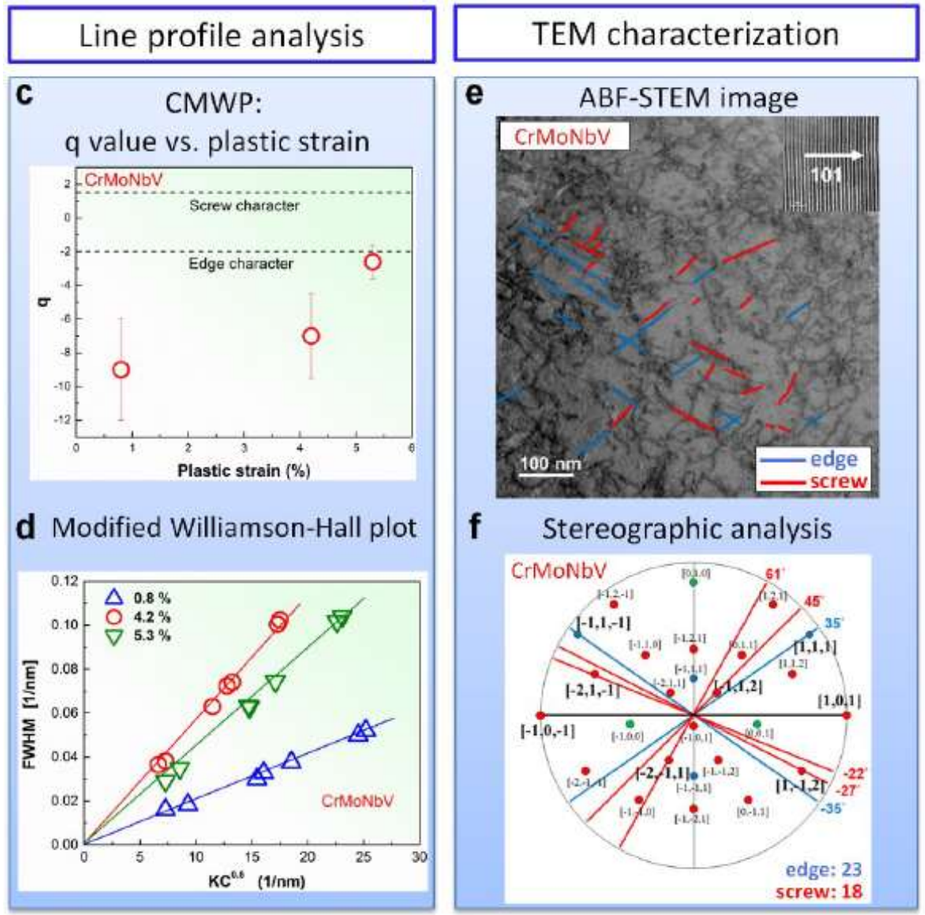
Maresca and Curtin (2020) Acta Mater 182, 235

Theory of strengthening: Edge dislocations in BCC alloys

NbTaTiV BCC High Entropy Alloy



CrMoNbV BCC High Entropy Alloy



Lee, Maresca et al. (2021) Nature Communications 12, 5474

Theory of strengthening: Edge dislocations in BCC alloys

$$\Delta \mathrm{E}^{tot}(\zeta, w)\ /L = \left[\kappa \frac{\Gamma w^2}{2\zeta} - \beta \left(\frac{\zeta}{2\sqrt{2}b}\right)^{\frac{1}{2}} \Delta \tilde{E}_p(w)\right] \frac{1}{(1+\kappa)\zeta}$$

E_L E_P

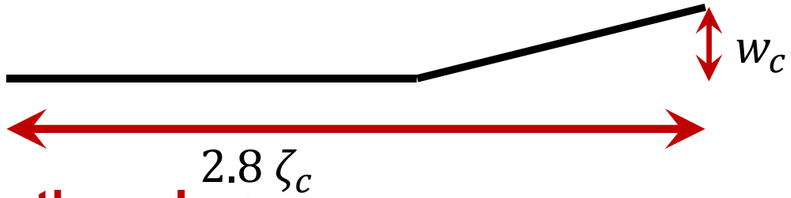
Total energy change per total length L

$\Gamma = \frac{1}{12}\mu b^2$ line tension

Minimizing w.r.t. ζ yields the penalization $E_L = \frac{1}{4}E_P$ (lower than screw case!).

Then, $\kappa = 0.56$ and $\beta = 0.83$ are determined self-consistently (numerically)

Repeating unit:



Characteristic **length scales**:

→ $\zeta_c = 1.727 \left(\frac{\Gamma^2 w^4 b}{\Delta \tilde{\mathrm{E}}_p^2(w)}\right)^{\frac{1}{3}}$ ζ_c and w_c from minimization of $\Delta \mathrm{E}^{tot}(\zeta, w)/\mathrm{L}$

Characteristic **energy barrier** in front of ζ_c segments:

→ $\Delta E_b = 1.11 \left(\frac{w_c^2 \Gamma \Delta \tilde{E}_p^2(w_c)}{b}\right)^{\frac{1}{3}}$ (from stochastic simulations)

Theory of strengthening: Edge dislocations in BCC alloys

One single strengthening mechanism!

Advancement of ζ_c segments over the energy barrier ΔE_b

Total energy barrier:

$$\longrightarrow \quad \Delta E(\tau) = \Delta E_b \left(1 - \frac{\tau}{\tau_{y0}}\right)^{\frac{3}{2}}$$

T=0K flow-stress

$$\tau_{y0} = \frac{\pi}{2} \frac{\Delta E_b}{b \zeta_c(w_c) w_c} = 1.01 \left(\frac{\Delta \tilde{E}_p^4(w_c)}{\Gamma b^5 w_c^5} \right)^{\frac{1}{3}}$$

Finite T, finite strain-rate flow stress

[Leyson, Curtin (2016) MSMSE 24, 065005]

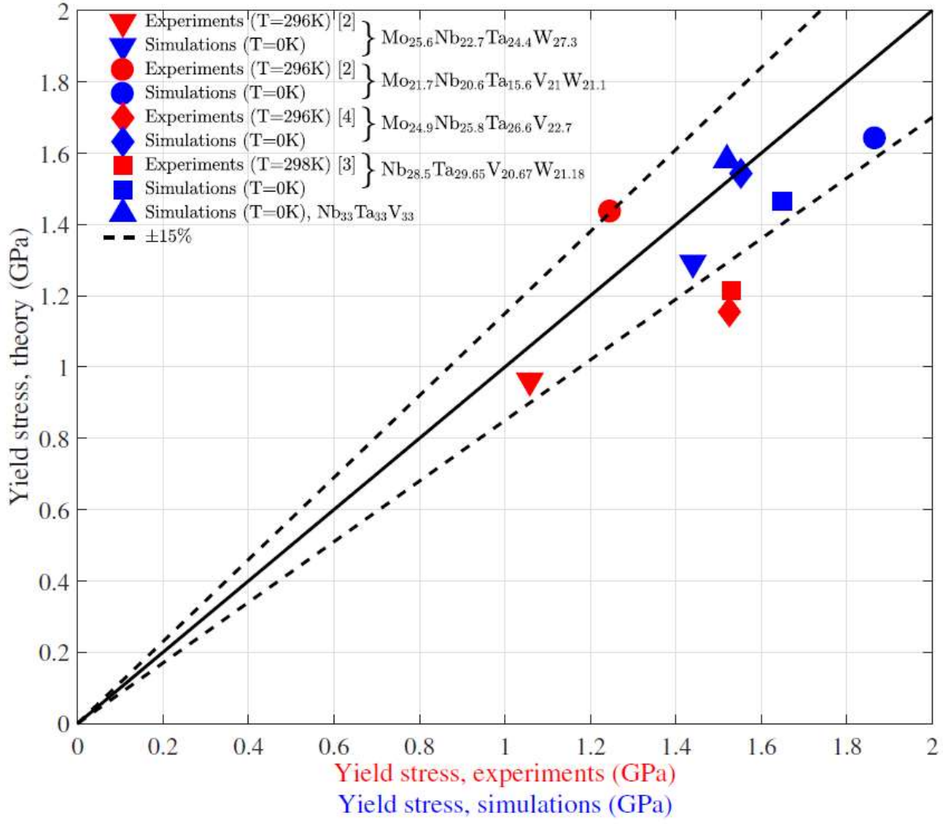
1) Low T $(\tau/\tau_{y0} > 0.5)$

$$\tau_y(T, \dot{\varepsilon}) = \tau_{y0} \left[1 - \left(\frac{kT}{\Delta E_b} \ln \frac{\dot{\varepsilon}_0}{\dot{\varepsilon}} \right)^{\frac{2}{3}} \right]$$

2) High T $(\tau/\tau_{y0} < 0.5)$

$$\tau_y(T, \dot{\varepsilon}) = \tau_{y0} \exp\left(-\frac{1}{0.55} \frac{kT}{\Delta E_b} \ln \frac{\dot{\varepsilon}_0}{\dot{\varepsilon}} \right)$$

Theory of strengthening: Edge dislocations in BCC alloys



Theory *vs* T=300K expts and MD simulations

Theory length-scales vs MD simulations

Mo-Nb-Ta-V-W	w_c theory (Å)	w_c simulations (Å)	$\lambda/4$ theory (Å)	$\lambda/4$ simulations (Å)
0.0-33.3-33.3-33.3-0.0	12.0	10.0	38.7	40.2
21.7-20.6-15.6-21-21.1	12.0	8.4	48.9	49.4
25.6-22.7-24.4-0.0-27.3	12.1	9.1	61.1	72.5
24.9-25.8-26.6-22.7-0.0	12.1	11.0	45.6	52.4
0.0-28.5-29.65-20.67-21.18	12.1	9.3	48.4	50.7

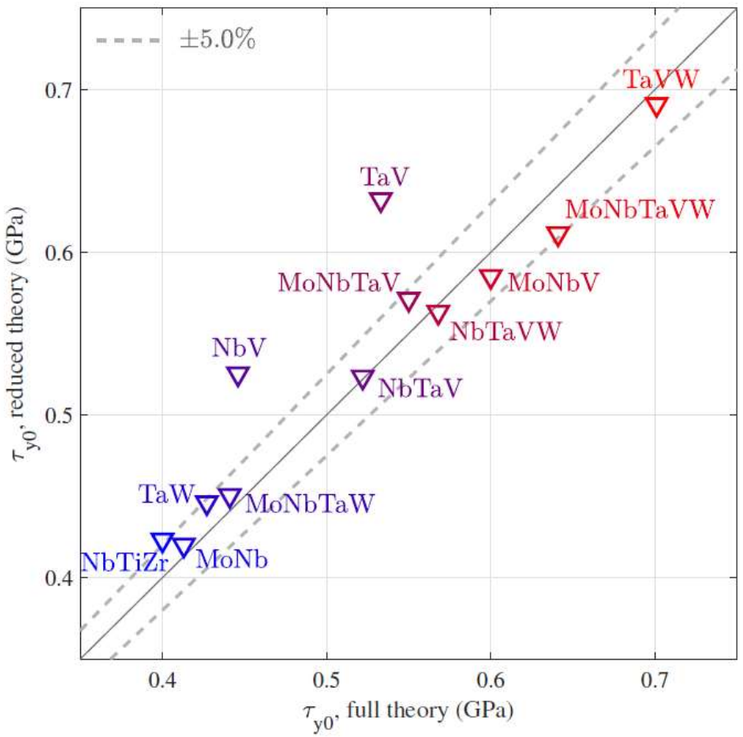
Theory of strengthening: Edge dislocations in BCC alloys

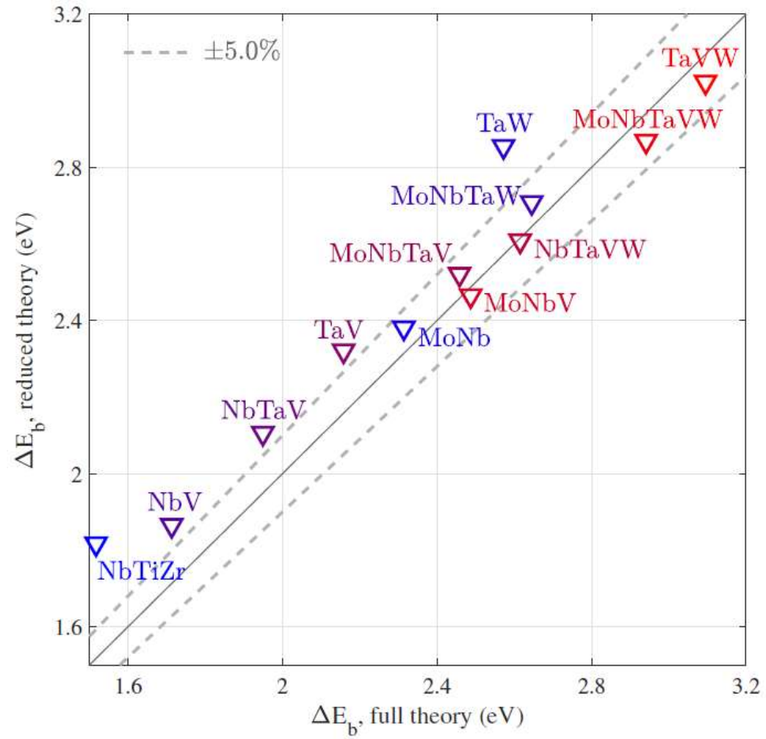
Analytic model for strengthening

$$\tau_{y0} = 0.040\alpha^{-\frac{1}{3}}\bar{\mu}\left(\frac{1+\bar{\nu}}{1-\bar{\nu}}\right)^{\frac{4}{3}}\left[\frac{\sum_n c_n \Delta V_n^2}{\bar{b}^6}\right]^{\frac{2}{3}}$$

$$\Delta E_b = 2.00\alpha^{\frac{1}{3}}\bar{\mu}\bar{b}^3\left(\frac{1+\bar{\nu}}{1-\bar{\nu}}\right)^{\frac{2}{3}}\left[\frac{\sum_n c_n \Delta V_n^2}{\bar{b}^6}\right]^{\frac{1}{3}}$$

$$\left(\Gamma = \alpha\mu b^2, \alpha = \left[\frac{1}{16}, \frac{1}{8}\right]\right)$$





Theory of strengthening: Edge dislocations in BCC alloys

Optimization performed over 10M compositions in Al-Cr-Mo-Nb-Ta-W-V-Ti-Zr-Hf

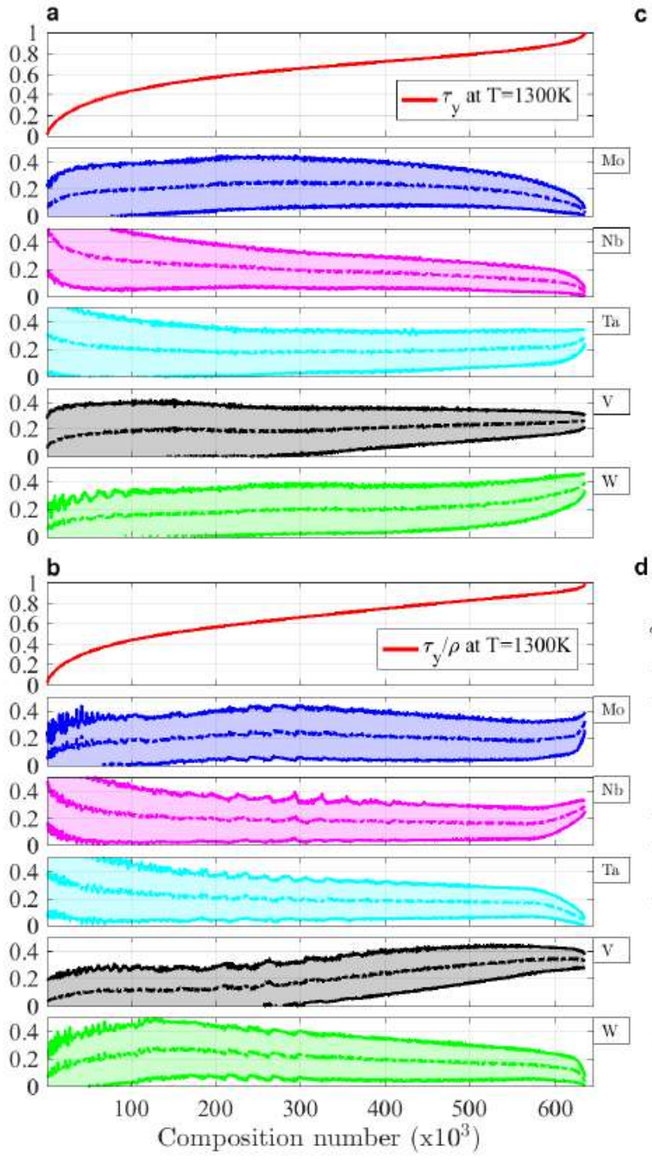
See:

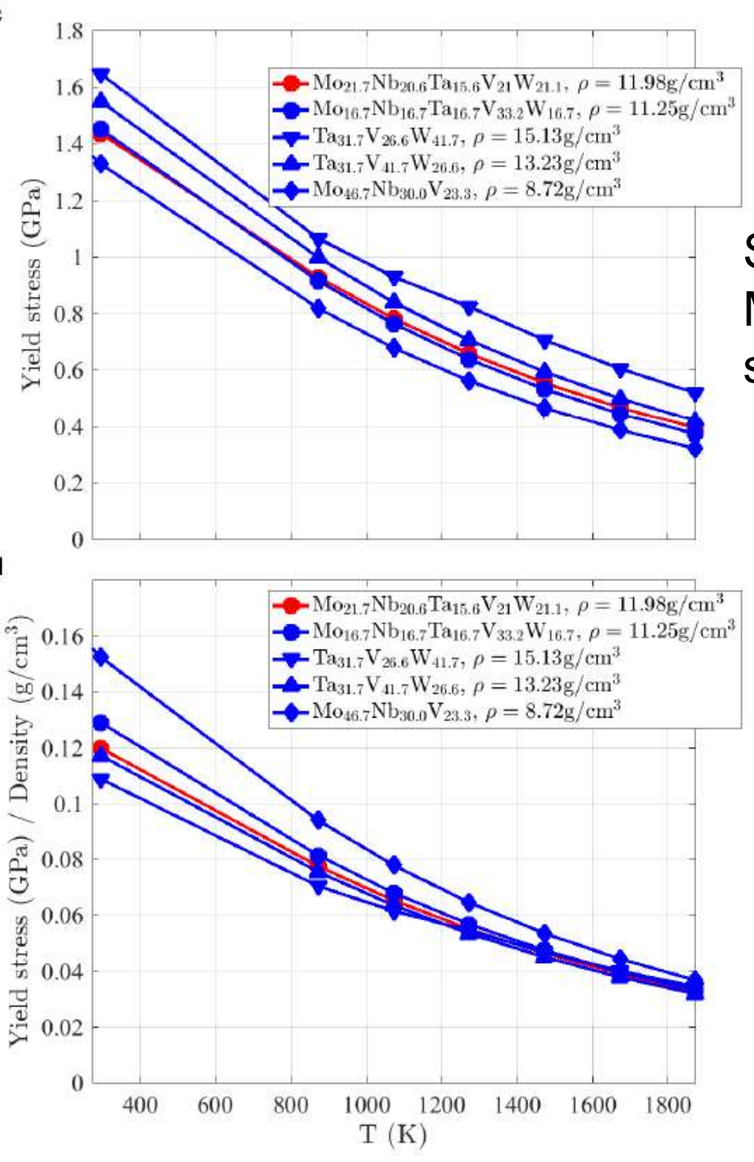
Lee, Maresca et al. (2021)
Nature Communications 12, 5474

MATLAB implementation available at

https://doi.org/10.24435/materialscloud:fs-27

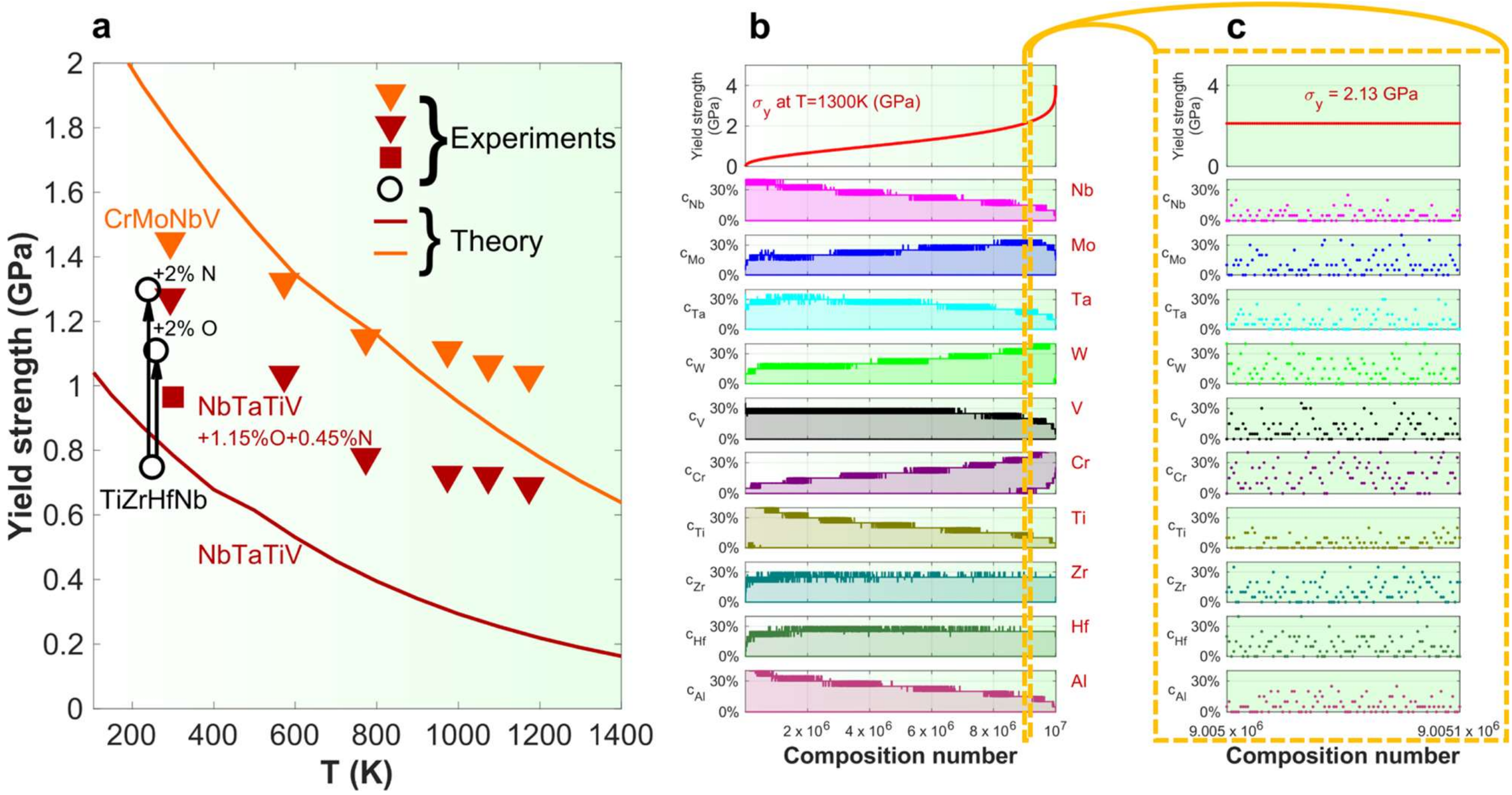
Taylor factor: 3.067





Shown here: Mo-Nb-Ta-V-W subset

Theory of strengthening: Edge dislocations in BCC alloys



Solid solution strengthening – F. Maresca (U. Groningen) Lee, Maresca et al. (2021) Nature Communications 12, 5474

Solid solution strengthening in BCC random alloys

Fully derived parameter-free theory for **screw and edge** strengthenig from dilute to “high entropy” alloys.

1) Minimum energy **screw dislocation is kinked** in alloys:
   x-kink strengthening controls high-T strength (up to Tm/2).

2) Edge strengthening rationalizes observed high-T strength
   in refractory BCC HEAs: xk-unpinning not operating above Tm/2.

3) Edge theory reduced to **simple form**, function of elastic moduli and volume misfits.

4) Theory used for **optimization** to find **new compositions** in immense BCC refractory alloys space.

Challenge: (Single-)phase predictions *ab-initio* [see Lee, Maresca et al. 2021; Ferrari, Lysogorskyi, Drautz (2021) PRM 5, 063606]

More details in:

Maresca & Curtin (2020) Mechanistic origin of high strength in refractory BCC high entropy alloys up to 1900K. *Acta Mater. 182:235*

Maresca & Curtin (2020) Theory of screw dislocation strengthening in random BCC alloys from dilute to “High-Entropy” alloys. *Acta Mater. 182:144*

Yin, Maresca & Curtin (2020) Vanadium is an optimal element for strengthening in both fcc and bcc high-entropy alloys. *Acta Mater. 188:486*

Ghafarollahi, Maresca & Curtin (2019) Solute/screw dislocation interaction energy parameter for strengthening in bcc dilute to high entropy alloys. *Modelling Simul. Mater. Sci. Eng. 27:085011*

Lee, Maresca, Feng, Chou, Ungar, Widom, An, Poplawski, Chou, Liaw, Curtin (2021) Strength can be controlled by edge dislocations in refractory high-entropy alloys. *Nature Communications 12:5474*