Ab-initio Cu alloy design for high-gradient accelerating structures

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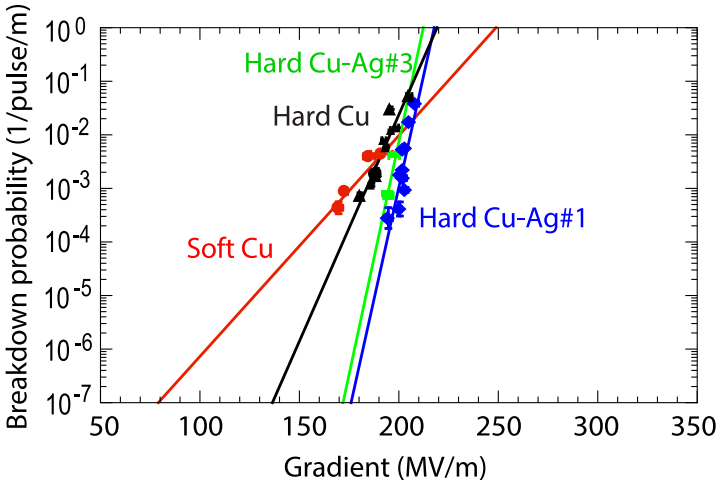
Outline

- Introduction
  - Figure of merit (FOM)
- Computational details
  - Compare calculated Cu alloy properties with existing experiments
- FOM of dilute Cu alloys
  - What alloy is good? At what solute concentration?
- Summary and plan

RF breakdown

- Breakdown probability is dependent on the material of the cavity.
- CuAg alloys can improve breakdown resistance
- Can we scan the whole periodic table in search of the optimal solute and concentration?



Simakov, Dolgashev, Tantawi, 2018

FOM overview

- Tradeoffs:
  - **Good:** Adding solute atoms can improve strength: limit plastic deformation under thermal loading
  - **Bad:** Adding solute atoms can increase RF dissipation and thermal stresses: increase driving force for plastic deformation

- **Figure of merit** (FOM):
  - Critical stress to move dislocations / Thermal stress created by RF dissipation

FOM #1: Critical stress to move dislocations

Labusch–Nabarro (LN) model: Critical resolved shear stress required for dislocation motion:

$$\tau_{L-N} = \frac{(2\omega f_m^4 c^2)^{1/3}}{2b^{7/3}(Gb^2)^{1/3}}$$

With: $f_m = \frac{Gb^2}{120}\varepsilon_L$ $\quad \varepsilon_L = \sqrt{\varepsilon_G'^{\,2} + (\alpha\varepsilon_b)^2}$ $\begin{cases} \alpha = 9 - 16 \\ \varepsilon_G' = \dfrac{\varepsilon_G}{1 + 0.5|\varepsilon_G|} \end{cases}$

Two key parameters:

- Size misfit $\varepsilon_b = \frac{db}{bdc}$
- Modulus misfit $\varepsilon_G = \frac{dG}{Gdc}$

Johan Zander et al., Computational Materials Science 41 (2007) 86–95
M. Z. Butt, Journal of Materials Science 28 (1993) 2557-2576

FOM #2: Thermal stress created by RF dissipation

- Heating due to RF losses can be estimated from the solution of the heat equation:

Accelerator parameters $\Delta T = \frac{G^2\sqrt{T_p}}{Z_H^2}\frac{R_s}{\sqrt{\pi\rho c_\varepsilon k}}$ Material properties

- Assuming that the surface is free to relax in z only, the corresponding in-plane thermal stress is

$$\varepsilon_{xx} \equiv \varepsilon_{yy} \equiv -\frac{E\alpha T}{1-v}$$

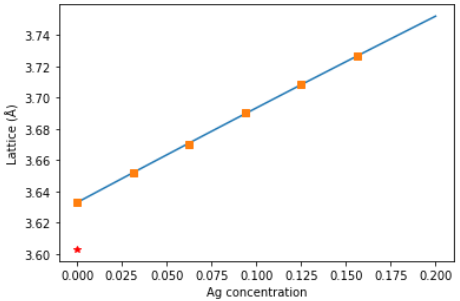
Perry B. Wilson. In ITP Conference on Future High Energy Colliders. University of California, Santa Barbara, October 1996.

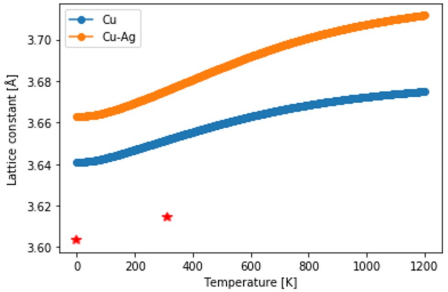
Calculating the FOM requires:

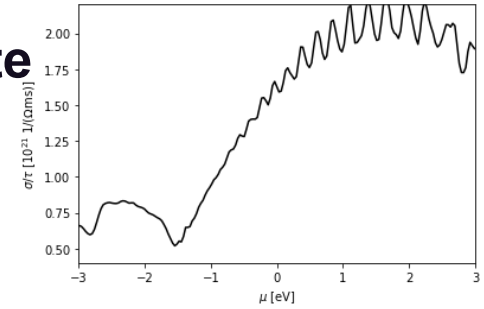
- Lattice constant: direct structure relaxation (DFT)
- Mechanical properties: finite distortion (DFT)
- Thermal expansion coefficient: quasi-harmonic approximation (DFT)
- Electrical and thermal conductivity:
  - SPRKKR

These quantities need to be computed vs solute concentration.

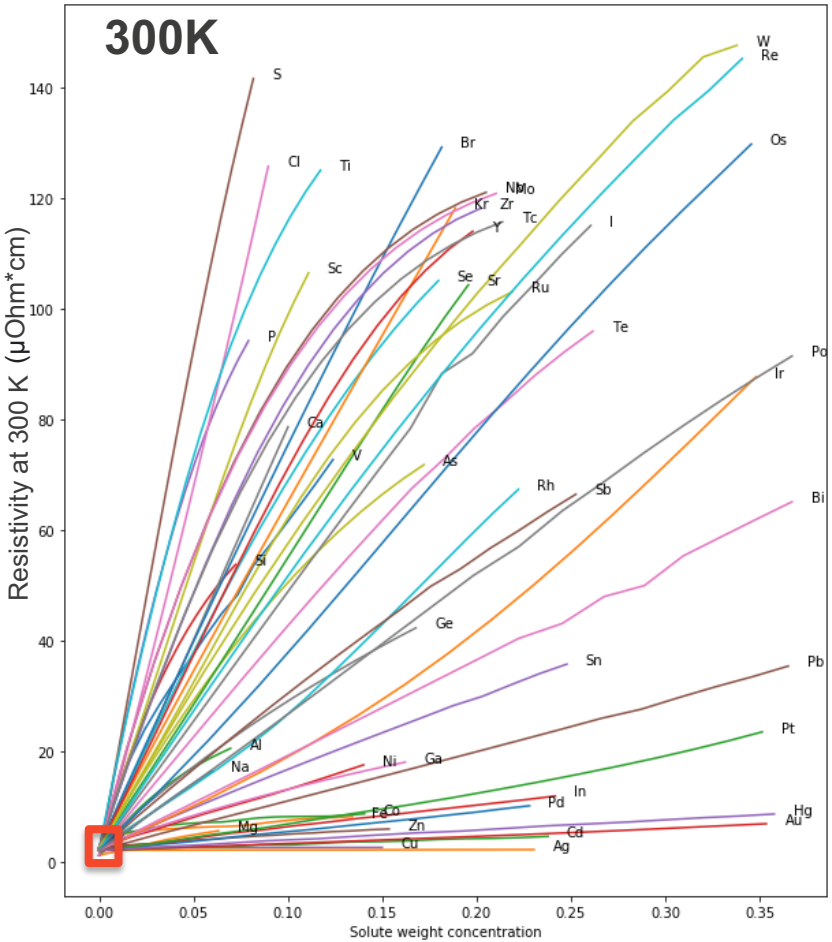
This requires tens of DFT calculations per solute per concentration (!)



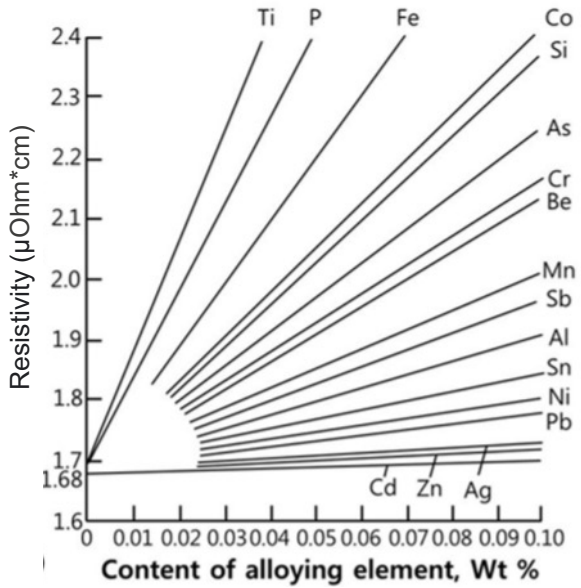




Resistivity

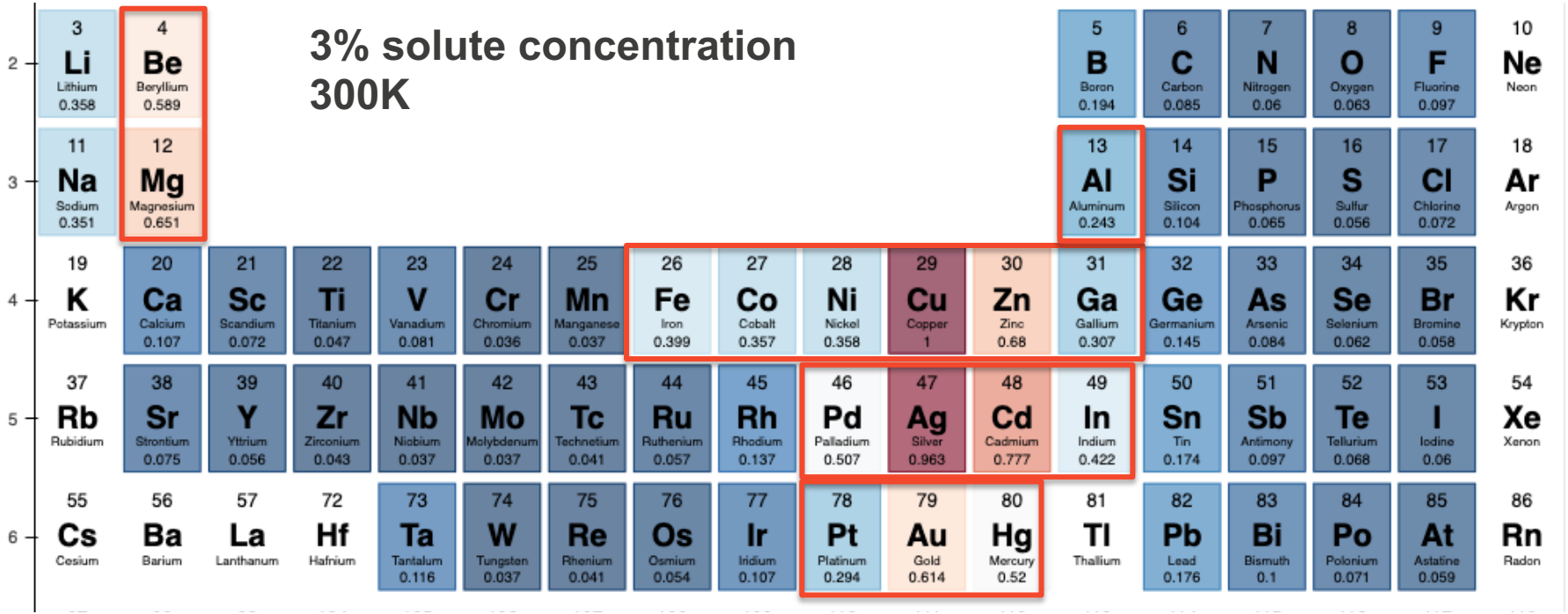


Experiments



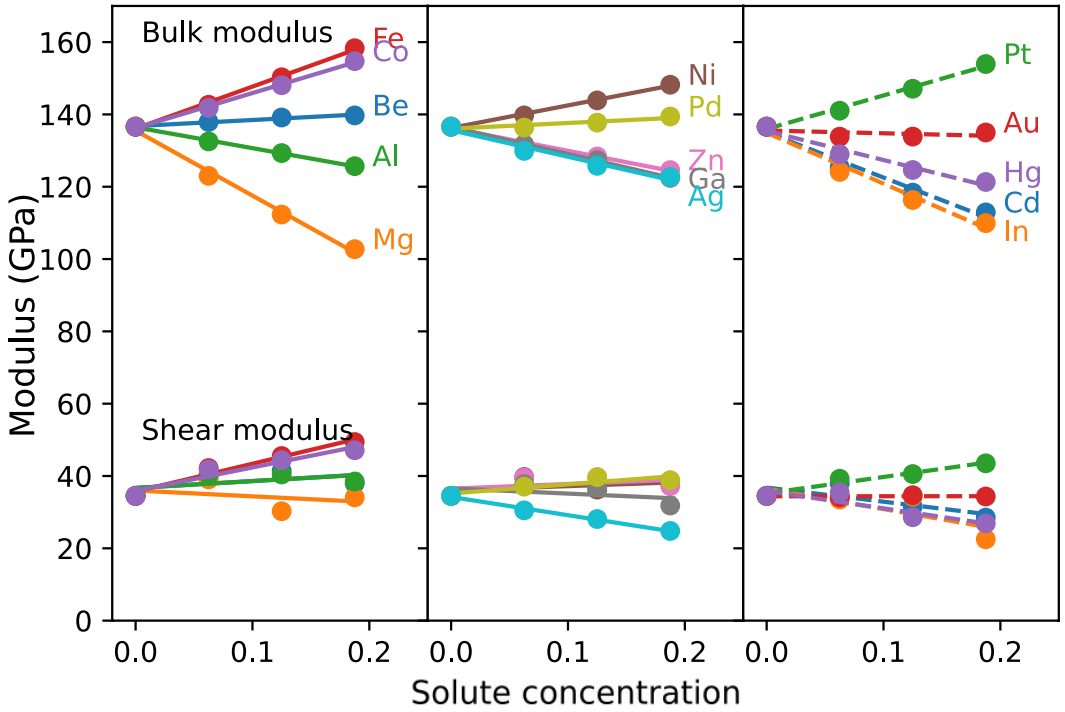
Experiments from: Han, Seung Zeon, Eun-Ae Choi, Sung Hwan Lim, Sangshik Kim, and Jehyun Lee. "Alloy design strategies to increase strength and its trade-offs together." *Progress in Materials Science* 117 (2021): 100720.

Electrical conductivity

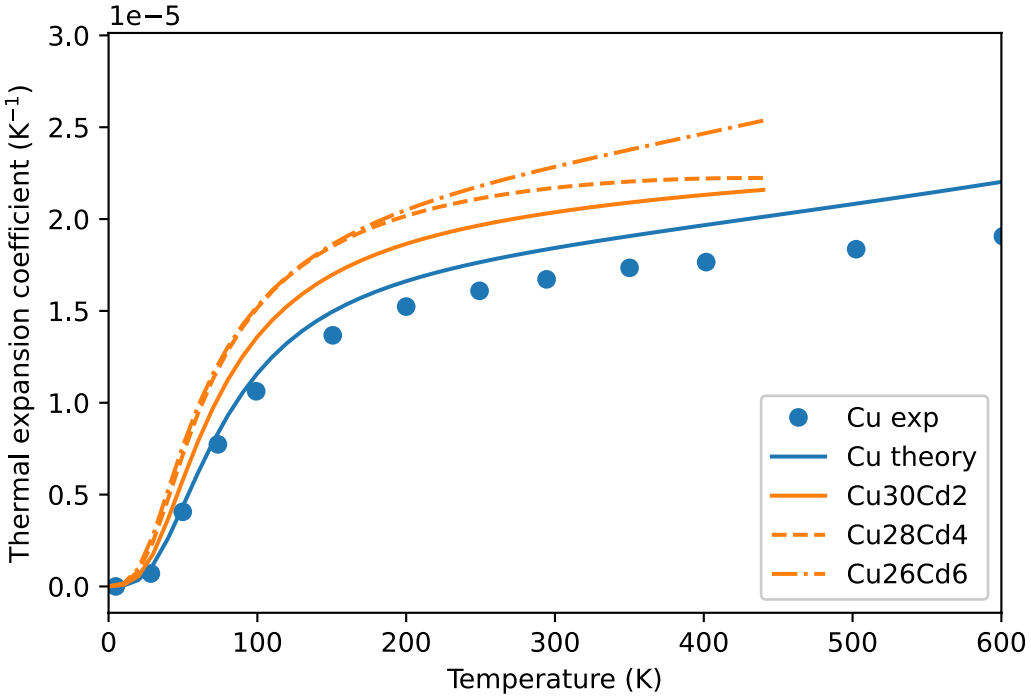


*(*Normalized by conductivity of pure Cu)*

Bulk and shear modulus

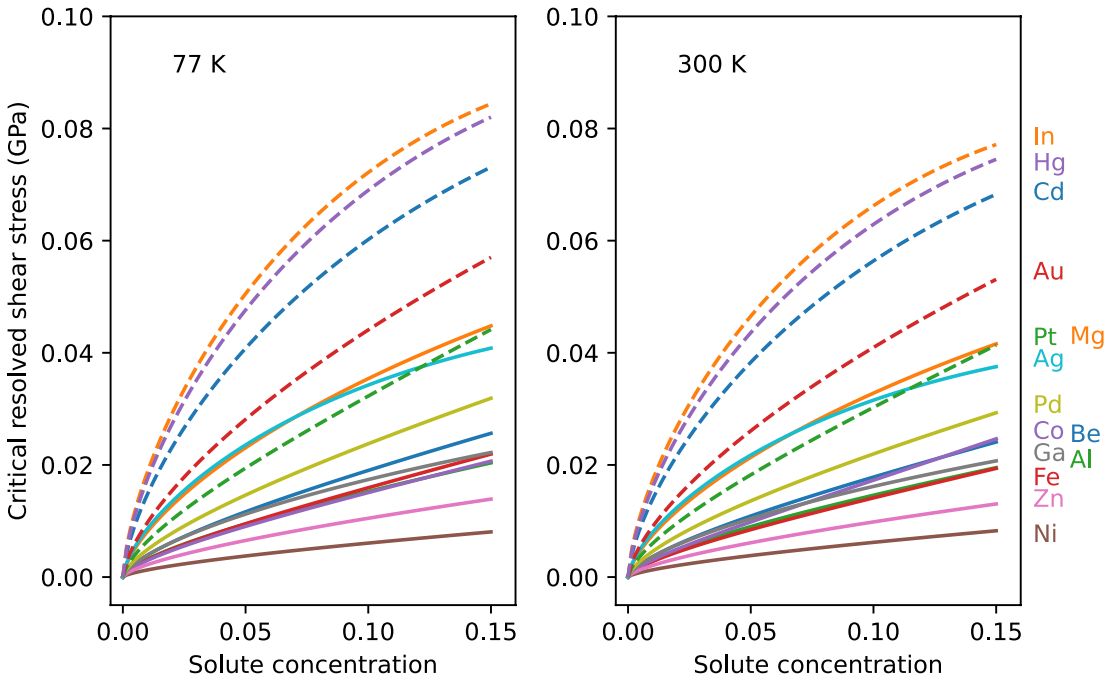


Thermal expansion coefficient



Experimental data from:
S. I. Novikova, Thermal expansion of solids (in Russian) (Nauka, Moscow, 1974).
D. V. Minakov et al., PHYSICAL REVIEW B 92, 224102 (2015)

FOM #1: Critical stress to move dislocations



$$\tau_{L-N} = \frac{(2\omega f_m^4 c^2)^{1/3}}{2b^{7/3}(Gb^2)^{1/3}}$$

$$\varepsilon_L = \sqrt{\varepsilon_G'^{\,2} + (\alpha\varepsilon_b)^2} \left\{ \begin{matrix} \alpha = 9 - 16 \\ \varepsilon_G' = \dfrac{\varepsilon_G}{1 + 0.5|\varepsilon_G|} \end{matrix} \right\}$$

$$\varepsilon_b = \frac{db}{bdc}$$

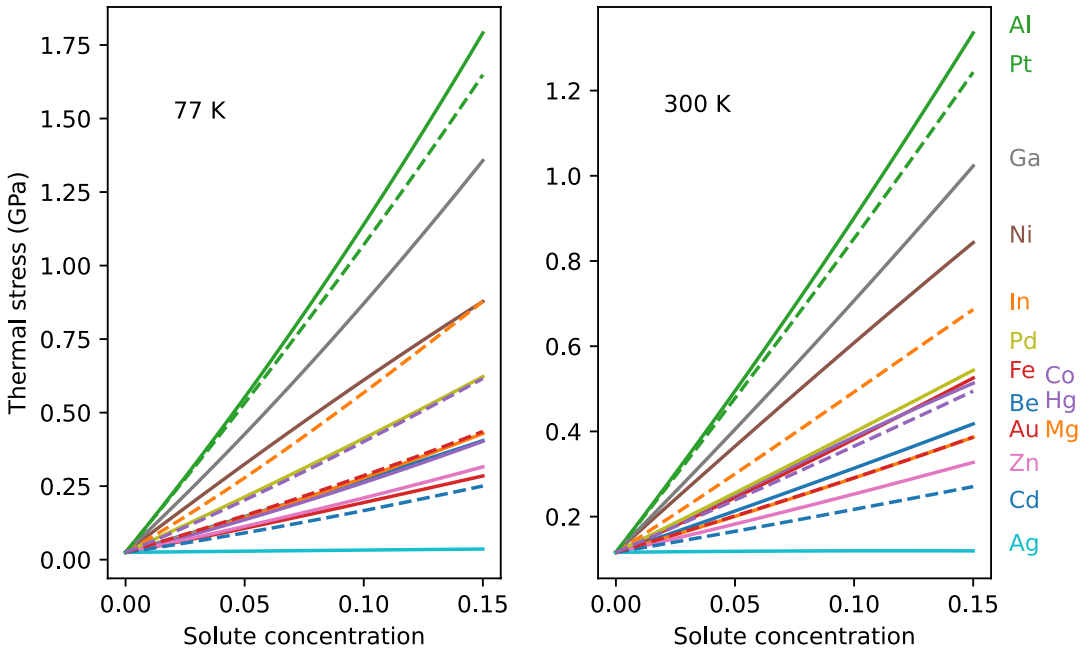
$$\varepsilon_G = \frac{dG}{Gdc}$$

$$G$$

$$b$$

Estimated from DFT calculations

FOM #2: Thermal stress created by RF dissipation



$$\varepsilon_{xx} \equiv \varepsilon_{yy} \equiv -\frac{E\alpha T}{1-\nu}$$

$$\Delta T = \frac{G^2\sqrt{T_p}}{Z_H^2}\frac{R_s}{\sqrt{\pi\rho c_\varepsilon \kappa}}$$

E
ν
ρ
α
c_ε

} Estimated from DFT calculations

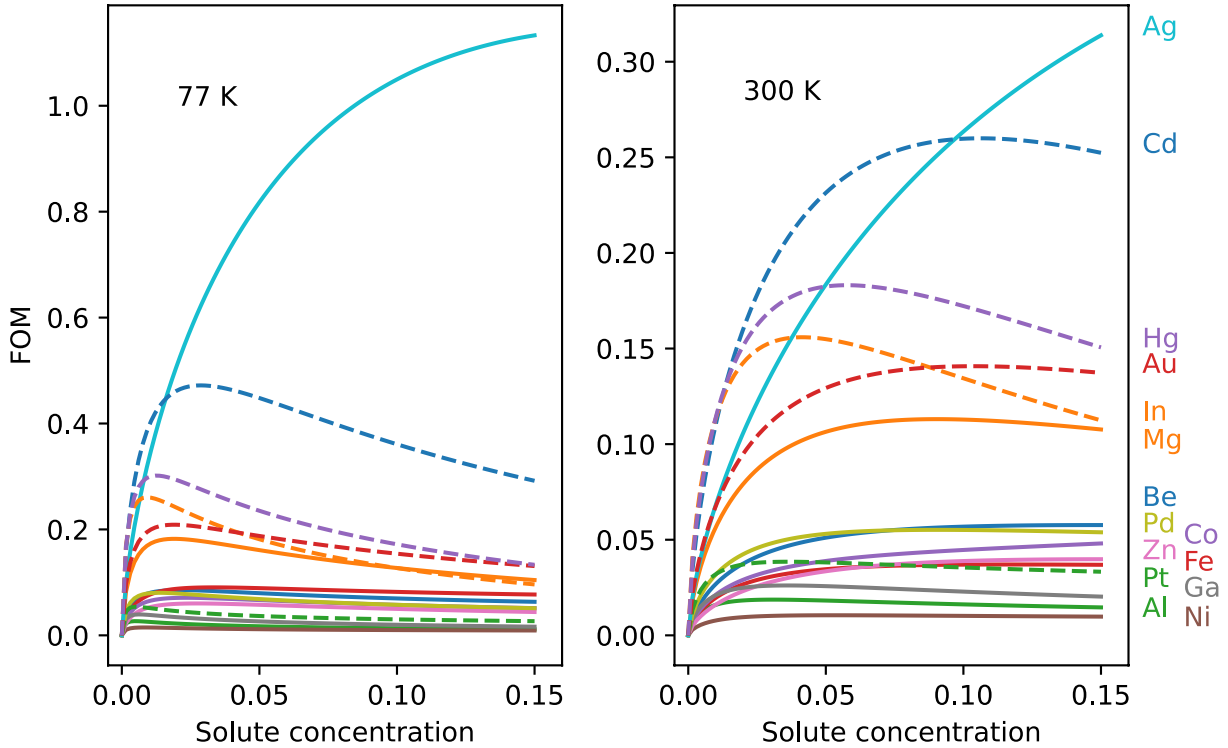
$$R_s = \sqrt{\frac{\pi\mu_0 c_{light}}{\lambda\sigma_c}}$$

k

} SPRKKR

$\frac{G^2\sqrt{T_p}}{Z_H^2}$ (unloaded gradient, RF pulse length, impedance)

FOM = FOM #1 / FOM #2



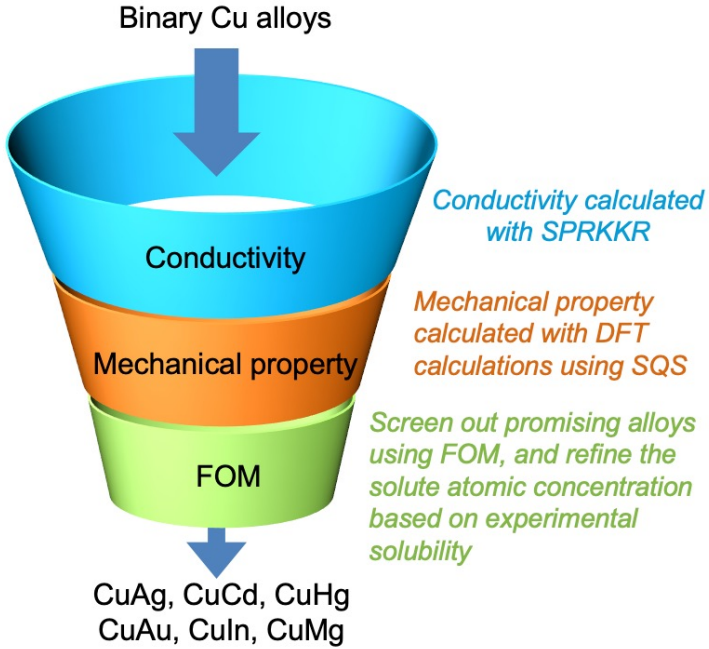
Summary and plan

Summary:

- FOM: tradeoff between solute strengthening and thermal stress
- Identify binary Cu alloys that are promising for high gradient accelerator design

Future work:

- Extend to ternary alloys
- Engage with experimental efforts to assess potential candidate alloys



- Wang, Gaoxue, Evgenya I. Simakov, and Danny Perez. *Applied Physics Letters* 120, no. 13 (2022): 134101.

Acknowledgements

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