Determining solute site preference and correlations to antiphase boundary energy in Ni-based superalloys

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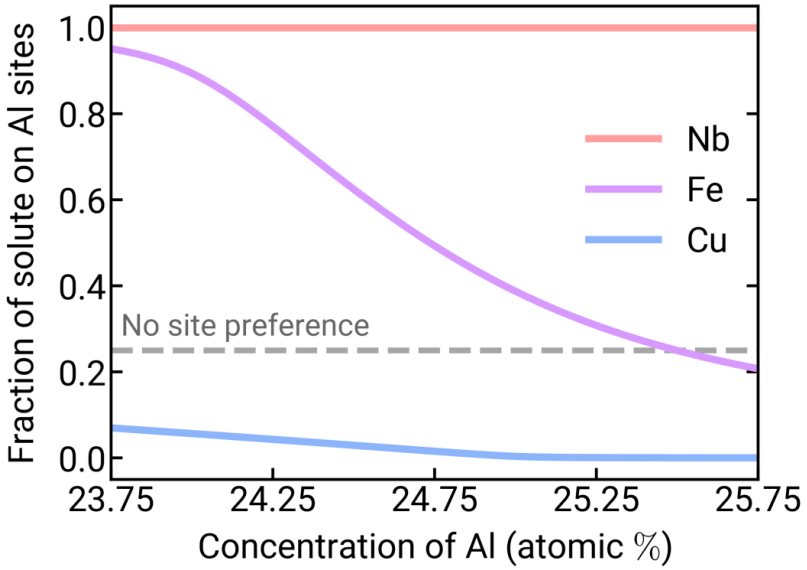

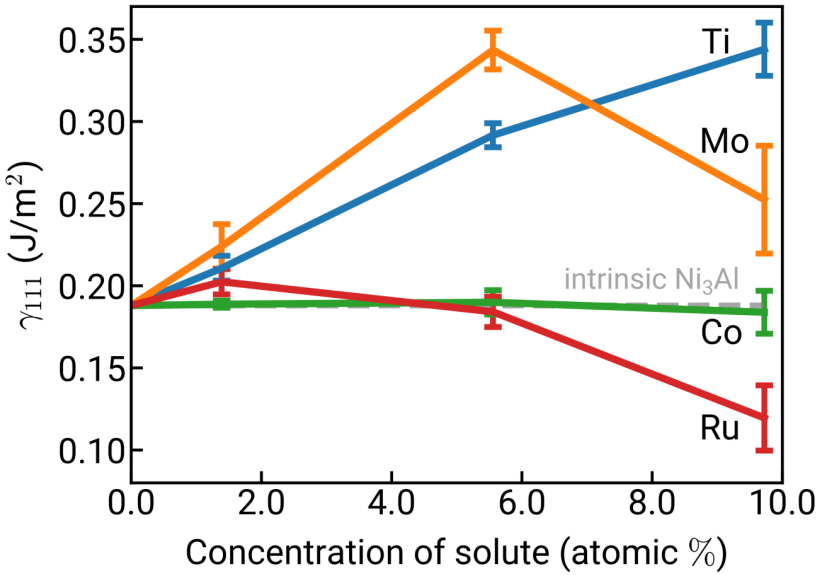

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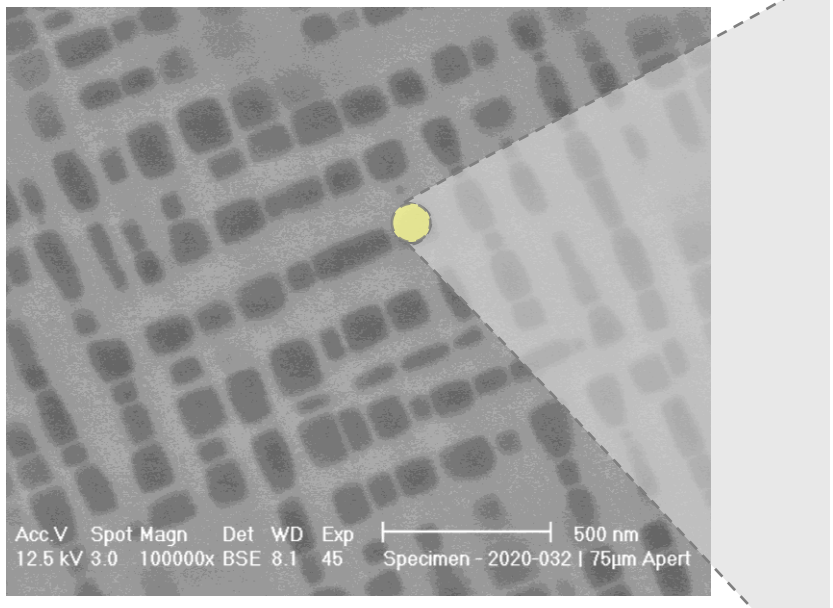
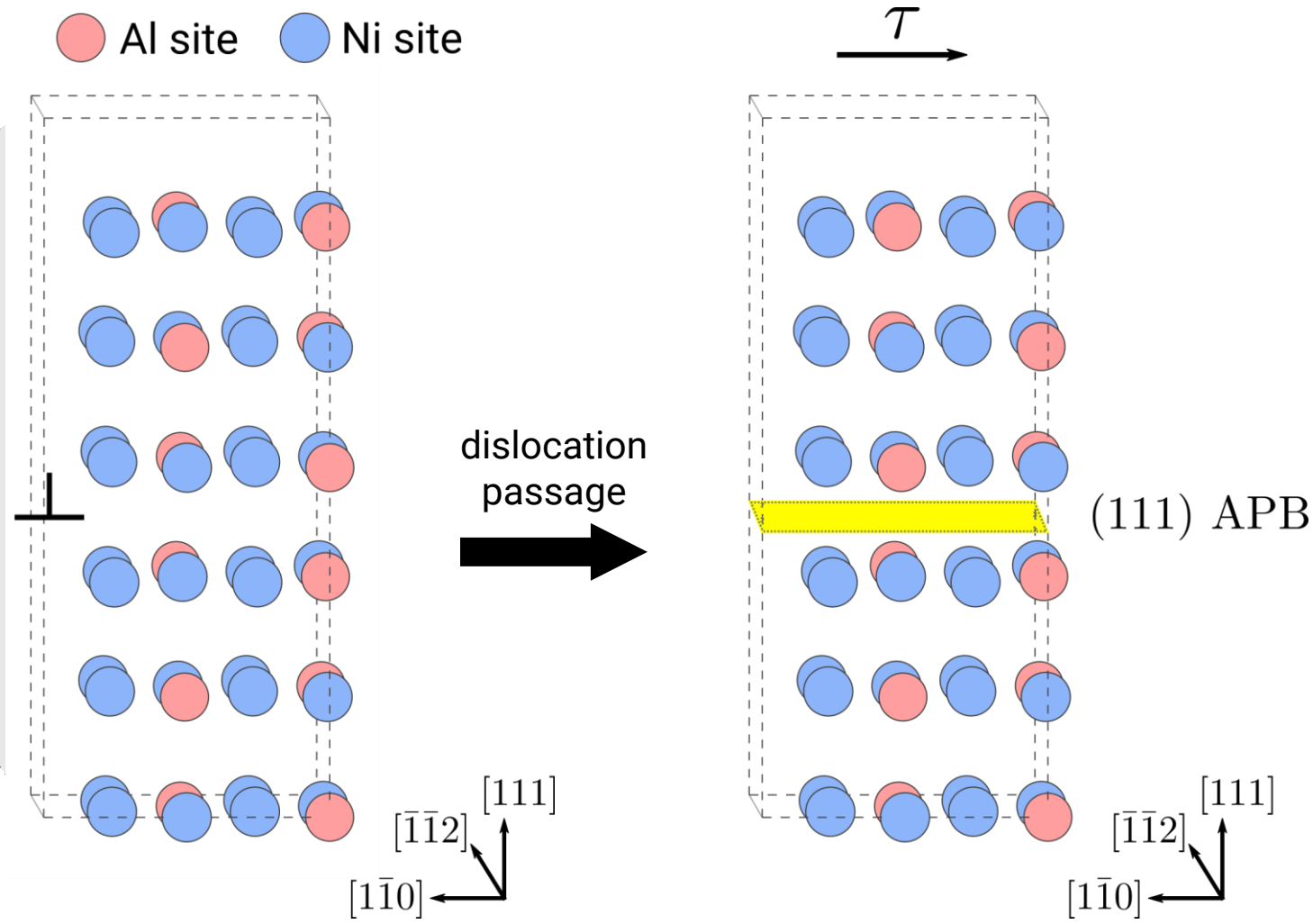
Superalloys and antiphase boundary (APB) energy





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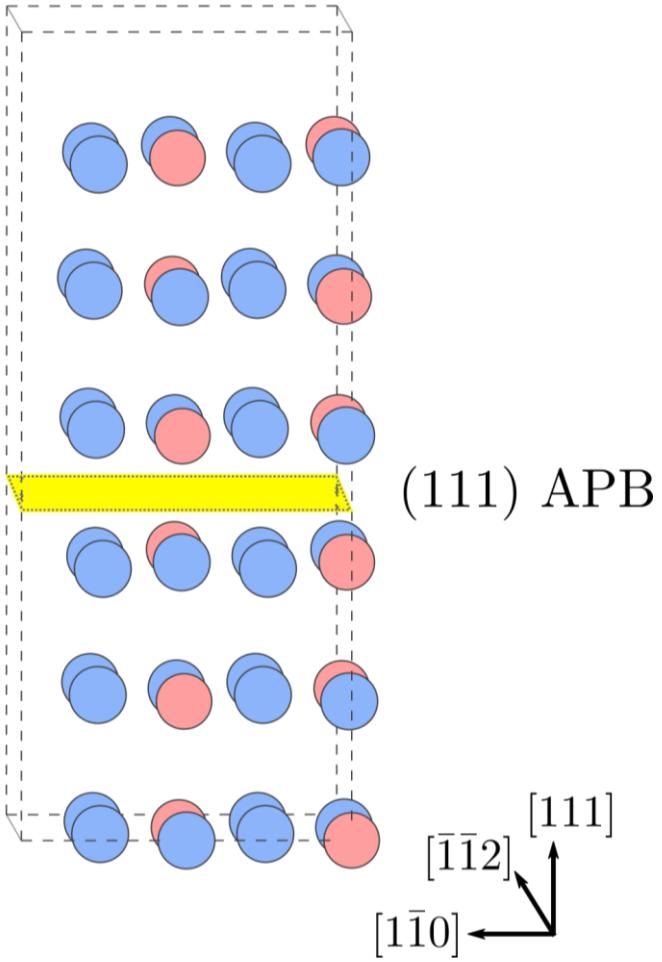

$$\sigma_{y_{\text{peak}}} \propto \frac{1}{2}\gamma_{\text{apb}} f^{1/2}/b$$

- f is the volume fraction of the precipitates
- b is the magnitude of the Burgers vector
- γ_{apb} is the APB energy

Reed, R.C. *The Superalloys*, Cambridge, 2006

Existing computational studies

- At low concentrations for several ternary species, the APB energy varies approximately linearly and monotonically with solute concentration [1,2].
- The APB energy is related to the ordering energy, with a particularly strong correlation for 3*d* transition metal solutes at low concentration [2].

[1] Crudden, D.J. et al. *Acta Materialia*, 2014
[2] Gorbatov, O.I. et al. *Phys. Rev. B*, 2016

Our methodology

- We implement automated workflows that accelerate data generation and analysis of the APB energy.
- We further look for correlations of APB energy with other physical properties.

1. Determine the site preference of solute species in Ni_3Al.
2. Calculate the APB energy in Ni_3Al-based alloys and analyze trends.
3. Identify correlations between physical properties and the APB energy.

Steps in our method

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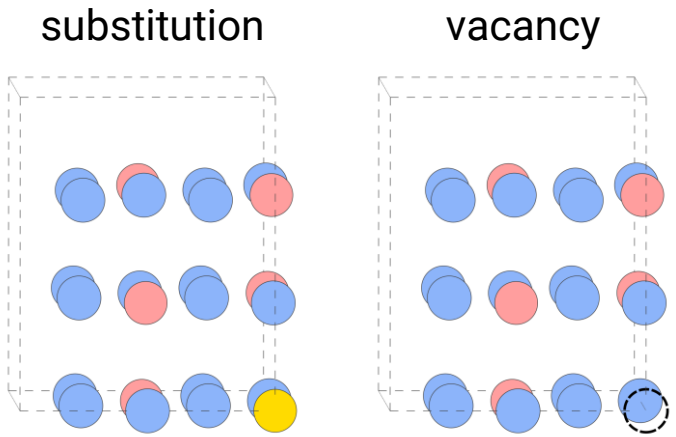
Solute site preference – DSM formalism

- Dilute solution model (DSM) with first-order low-temperature expansion [1].

$$\Omega = E^0 - \sum_i \mu_i \sum_p \lambda(p) c_i^0(p) - k_B T \sum_p \lambda(p) \sum_\epsilon \exp\left(- \left[\delta E^\epsilon(p) - \sum_i \mu_i \delta c_i^\epsilon(p) \right] \Big/ k_B T \right)$$

$$\langle c_i(p) \rangle = c_i^0(p) + \sum_\epsilon \delta c_i^\epsilon(p) \exp\left(- \left[\delta E^\epsilon(p) - \sum_j \mu_j \delta c_j^\epsilon(p) \right] \Big/ k_B T \right)$$

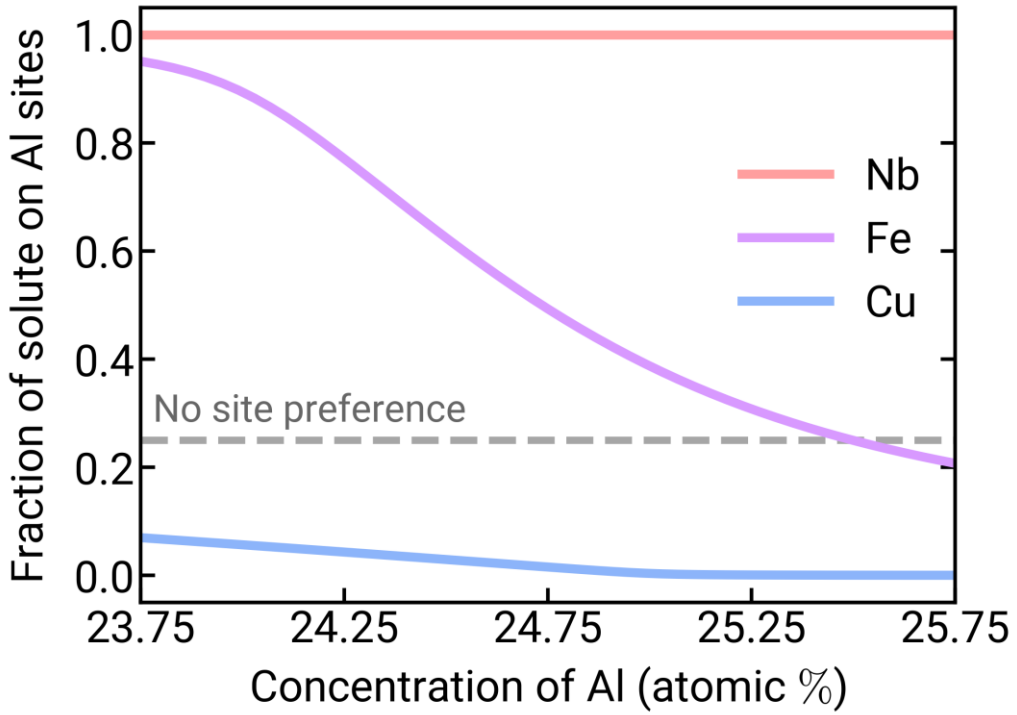
- Implemented in PyDII [2].

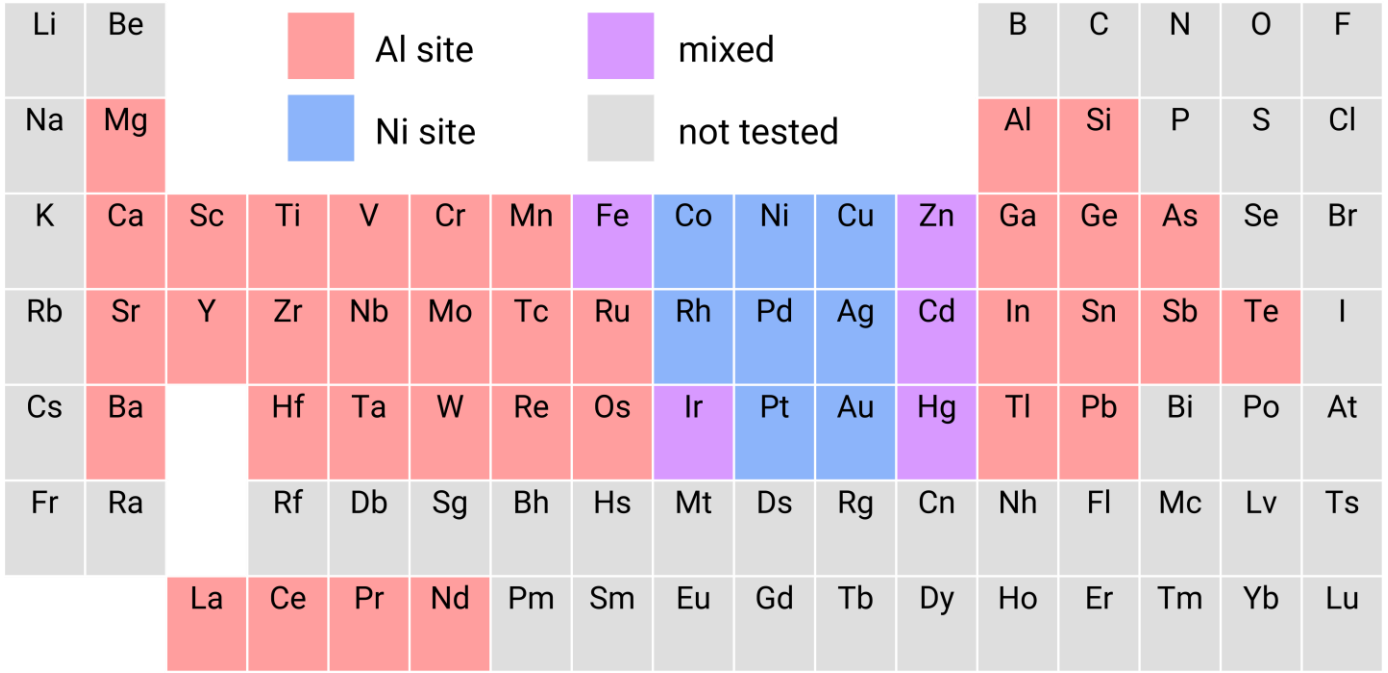


[1] Woodward, C. et al. *Phys. Rev. B*, 2001
[2] Ding, H. et al. *Comp. Phys. Comm.*, 2015; GitHub

Solute site preference - PyDII results

$$f_i(\mathrm{Al}) = \frac{\langle c_i(\mathrm{Al})\rangle}{\langle c_i(\mathrm{Al})\rangle + 3\langle c_i(\mathrm{Ni})\rangle}$$





Sublattice preference in Ni_3Al agrees with
Jiang, C. and Gleeson, B. *Scripta Materialia*, 2006

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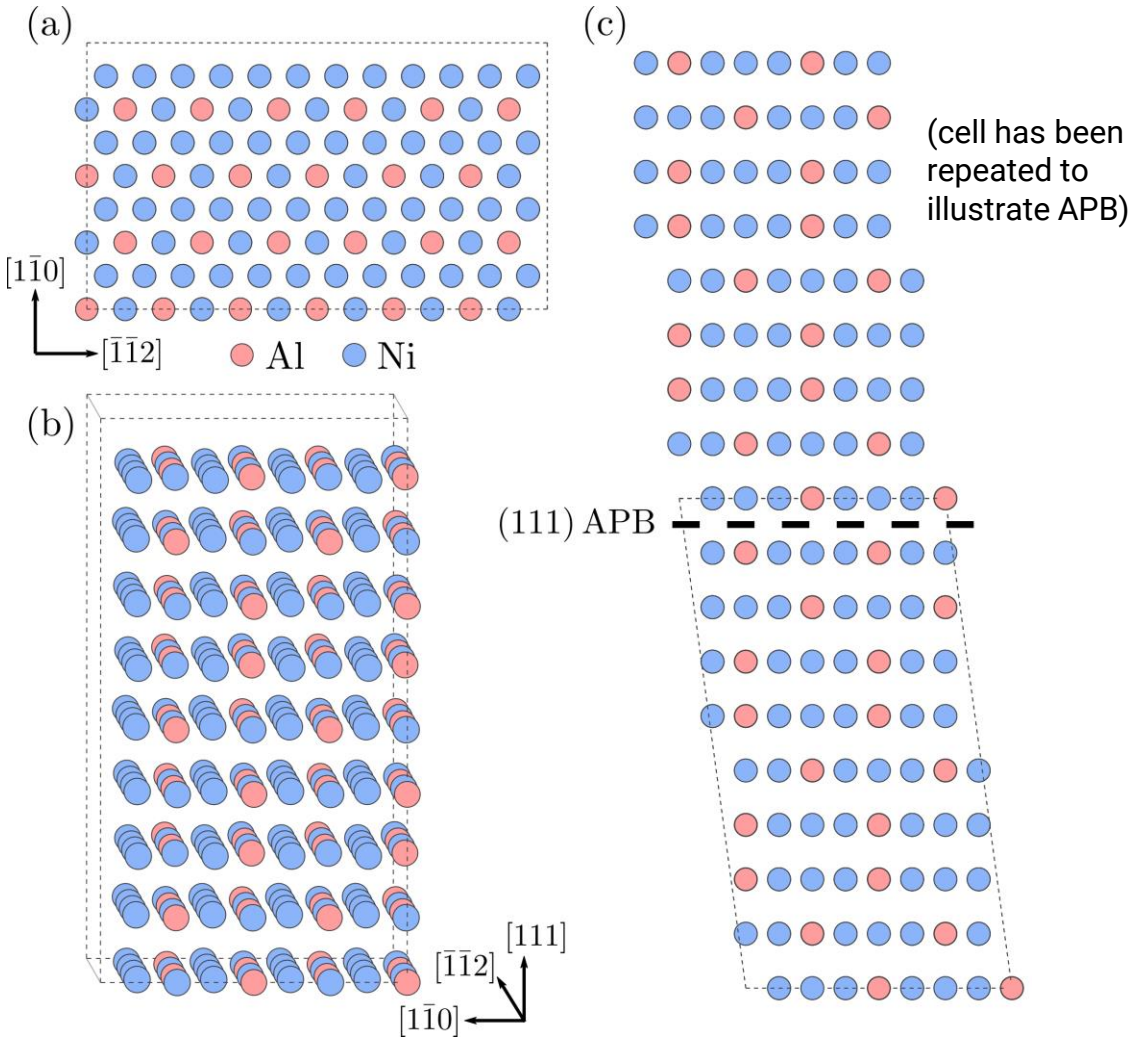
DFT calculations for γ_{111}

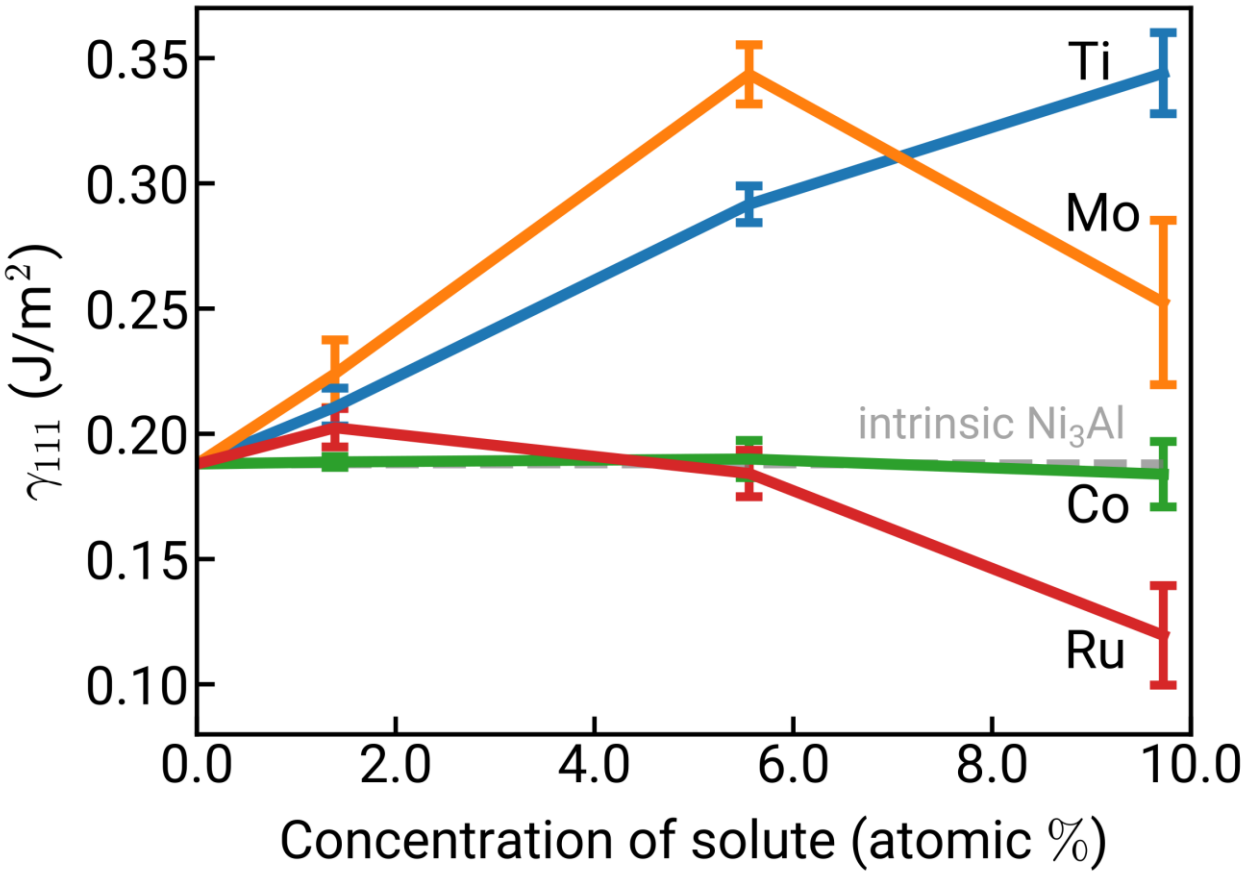
- 288-atom supercells with *z*-axis parallel to the [111] direction. Tilt creates an APB.
- At three concentrations for 30+ ternary elements, we randomly place solutes on the sublattice calculated by PyDII.

$$\gamma_{111} = \frac{E_{\text{apb}} - E_{\text{bulk}}}{A_{111}}$$



Representative γ_{111} vs. concentration profiles

- Most alloys with solutes that prefer the Al sublattice increase γ_{111} with increasing concentration.
- Elements with Ni or mixed sublattice preference tend to have little effect or decrease γ_{111}.
- Some are noticeably non-monotonic, such as solutes in groups 6 and 7.



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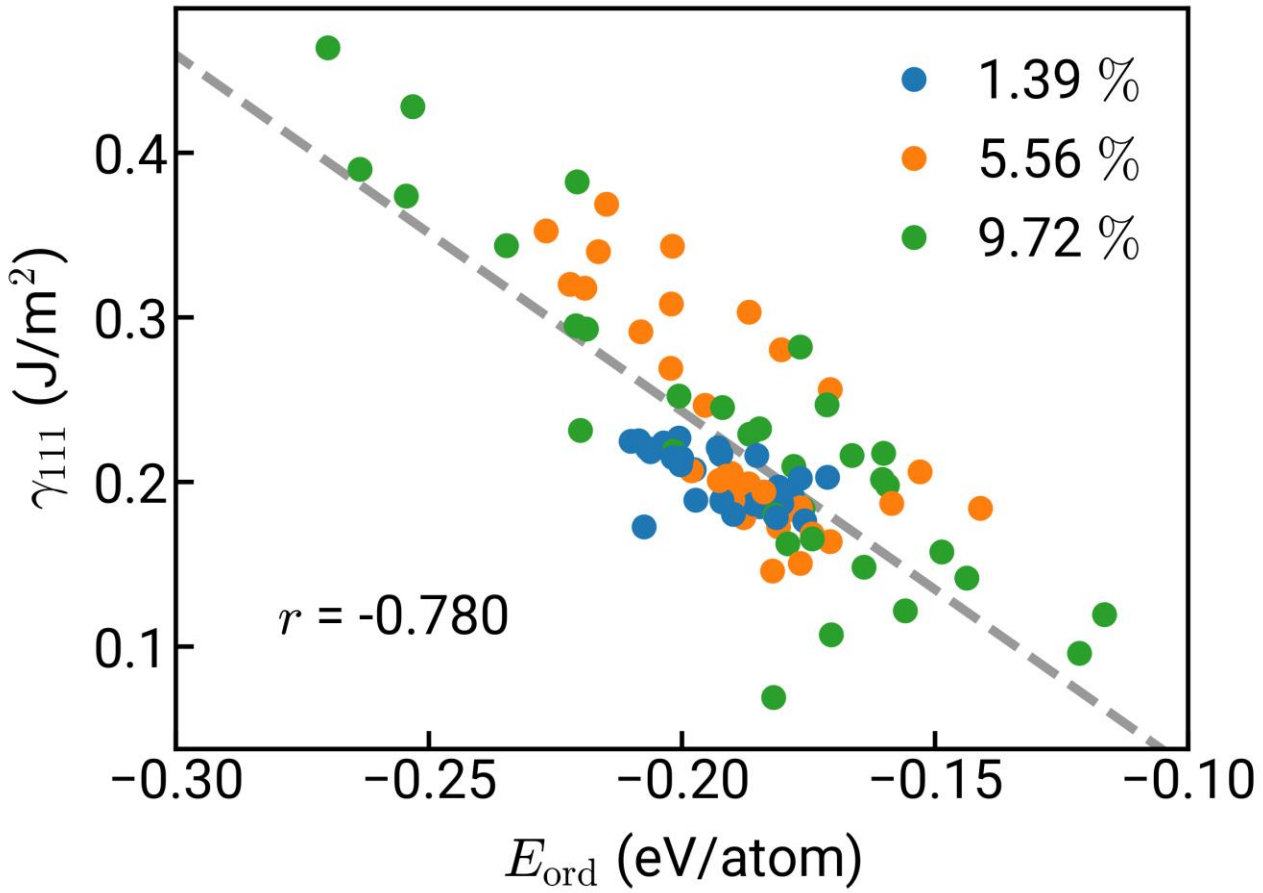
Correlation of γ_{111} with ordering energy (E_{ord})

$$E_{\mathrm{ord}} = \frac{E_{\mathrm{bulk}} - E_{\mathrm{random}}}{N}$$

- We find a moderately strong linear correlation between γ_{111} and E_{ord}.
- E_{ord} can also be calculated using CALPHAD methods [1].



[1] Miodownik, A. and Saunders, A. *TMS*, 1995

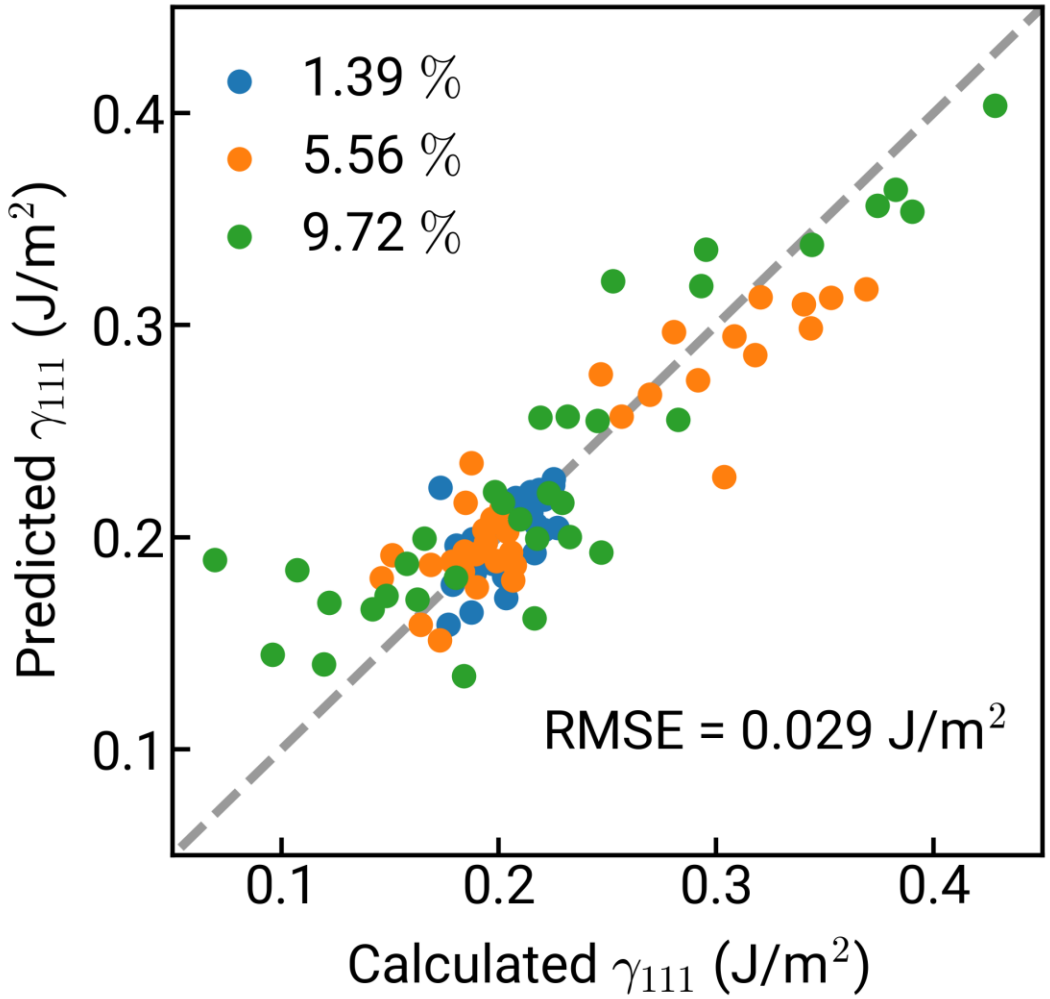
Feature engineering for machine learning (ML)

- We use Magpie and Matminer libraries [1] to generate more physical descriptors that are composition-weighted averages of the elemental properties.
- We calculate the permutation importance of the features [2]:
  1. Ordering energy
  2. Mean Pettifor number
  3. Mean number of unfilled orbitals
  4. Mean space group number
  5. Mean column number
- After cross-validation (CV) we select only the top 7 features for model building.

[1] Ward, L. et al. *npj Comp. Mater.*, 2016; Ward, L. et al. *Comp. Mater. Sci.*, 2018
[2] Breiman, L. *Machine Learning*, 2001

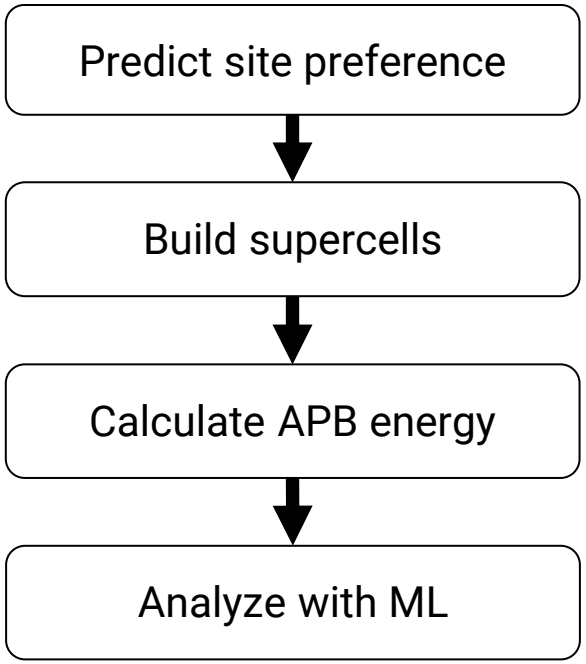
Predicting γ_{111} with an ML model

- We use the random forest ML model in Scikit-learn [1].
- We perform grouped 5-fold CV and calculate the average RMSE.

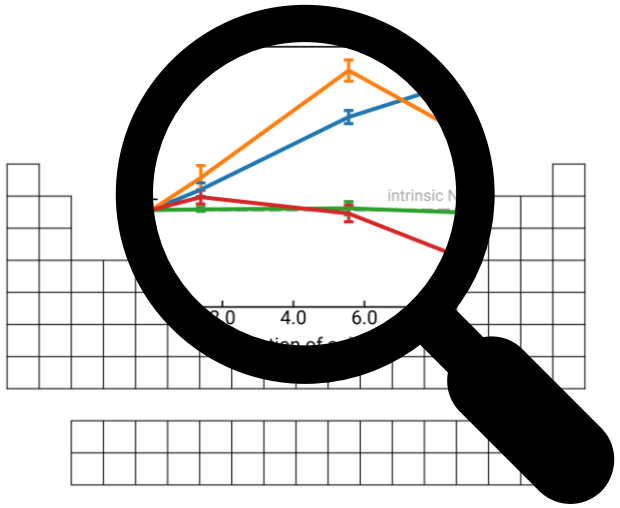


[1] Pedregosa, F. et al. *JMLR*, 2011

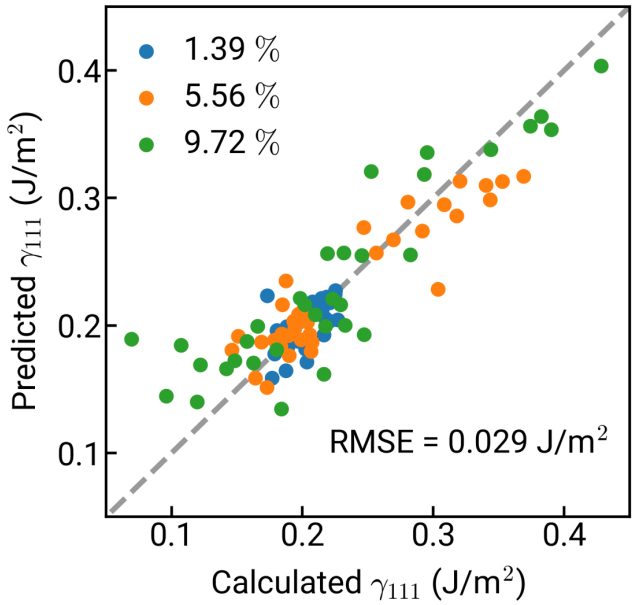
Conclusions



Created workflows to automate calculations



Analyzed trends in APB energy



Generated features for predictive ML models

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