First-principles and Data-driven Discovery of High-entropy Alloys for Corrosion Protection

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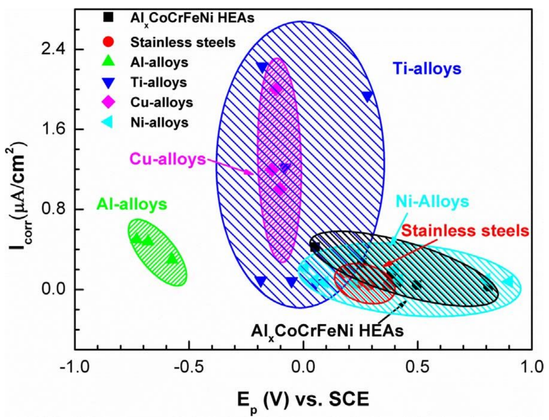
Introduction

Corrosion performance by alloy types [1]



Background & Motivation

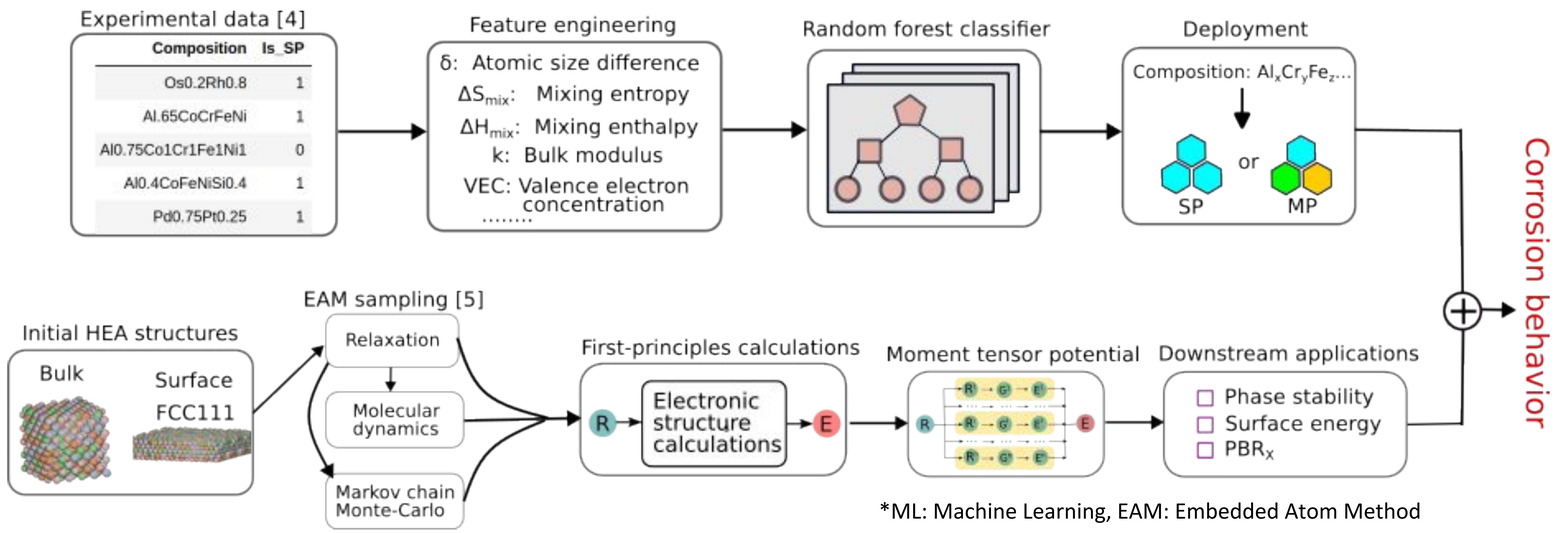
- Corrosion costs a lot.
- High-entropy alloys (HEA) are superior for corrosion protection.

Challenges

- HEAs live in high-dimensional search space.
- Unclear relation between compositions and corrosion behavior.

➔ **Machine learning accelerated search of corrosion-resistant HEAs**

Workflow for ML-enabled discovery of corrosion-resistant HEA

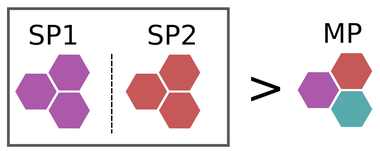


*ML: Machine Learning, EAM: Embedded Atom Method

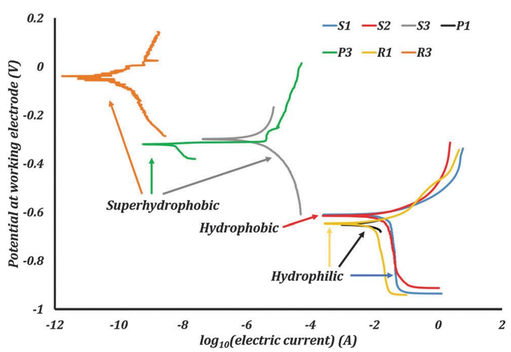
Three factors influencing corrosion

Phase type and stability

Single-phase (SP) is better than multiple-phase (MP)



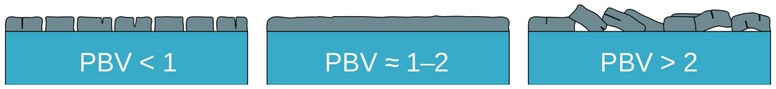
Surface energy [2]



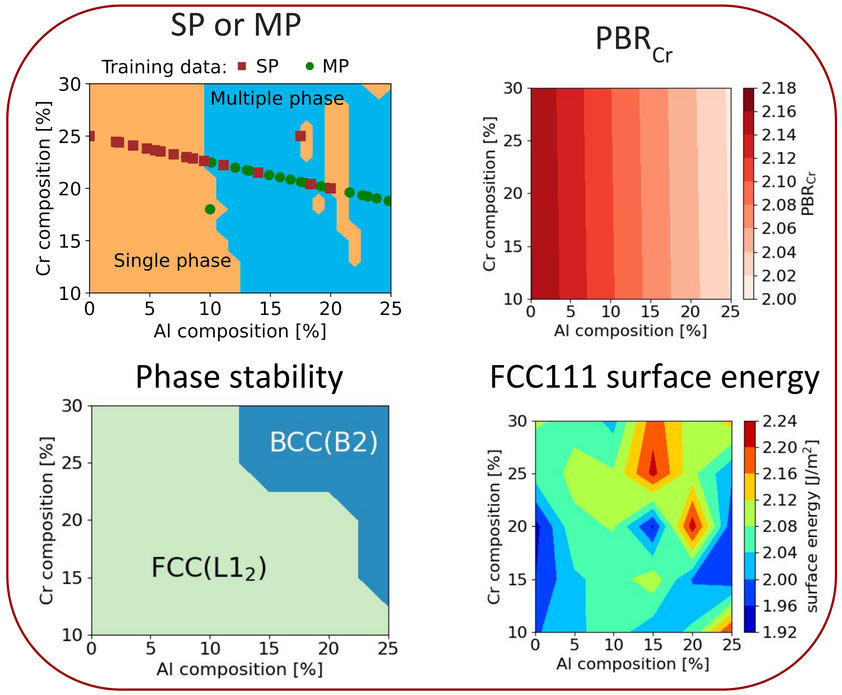
$$\frac{I_{(h,k,l)}}{I_{(m,n,p)}} = \exp\left\{\frac{\alpha(\gamma^{(h,k,l)} - \gamma^{(m,n,p)})}{RT}\right\}$$

Pilling-Bedworth Ratio (PBR) for oxidation of alloys [3]

$$PBR_{\text{alloy}} = \frac{\text{Volume of a mole of } B_xO_y}{\text{Volume of x moles of B in alloy}}$$



Synergistic effects of Al and Cr for $Al_xCr_yFeNiCo$



- Al is the critical element and Cr is the associated element.
- Low Al and Cr compositions tend to show single phase, FCC structure, high PBR_{Cr} (>2) and low FCC111 surface energy.
- The best combo is around **(Al, Cr)=(0, 15-18%)**.

Conclusions

- A framework combining first-principles calculations and data-driven models to evaluate corrosion performance of HEAs is developed.
- Corrosion behavior is gauged in terms of SP formability, PBR and surface energy.
- SP formability is predicted by random forest classifier and the other properties are quantified by moment tensor potential.
- For $Al_xCr_yFeNiCo$, the best Al and Cr composition ranges are around 0% and 15-18%.

References

[1] Shi et al., *Corrosion Science*, 133, 2018.
[2] Ramachandran and Nosonovsky, *Phys. Chem. Chem. Phys.*, 17, 2015.
[3] Xu and Gao, *Mat. Res. Innovzat.*, *3*(4), 2000.
[4] Yan et al., *Comput. Mater. Sci.*, 199, 2021.
[5] Farkas and Carlo, *J. Mater. Res.*, 35(22), 2020.
[6] A. V. Shapeev, *Multiscale Model. Simul.*, 14(3), 2016.