Design of Metal Alloys via Machine Learning Methods

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Metal Alloys for Aerospace Applications

http://aerospacelegacyfoundation.com/

https://spinoff.nasa.gov/Spinoff2015/ip_4.html

Ni-Ti alloys as hard bearing materials

Multicomponent Alloys

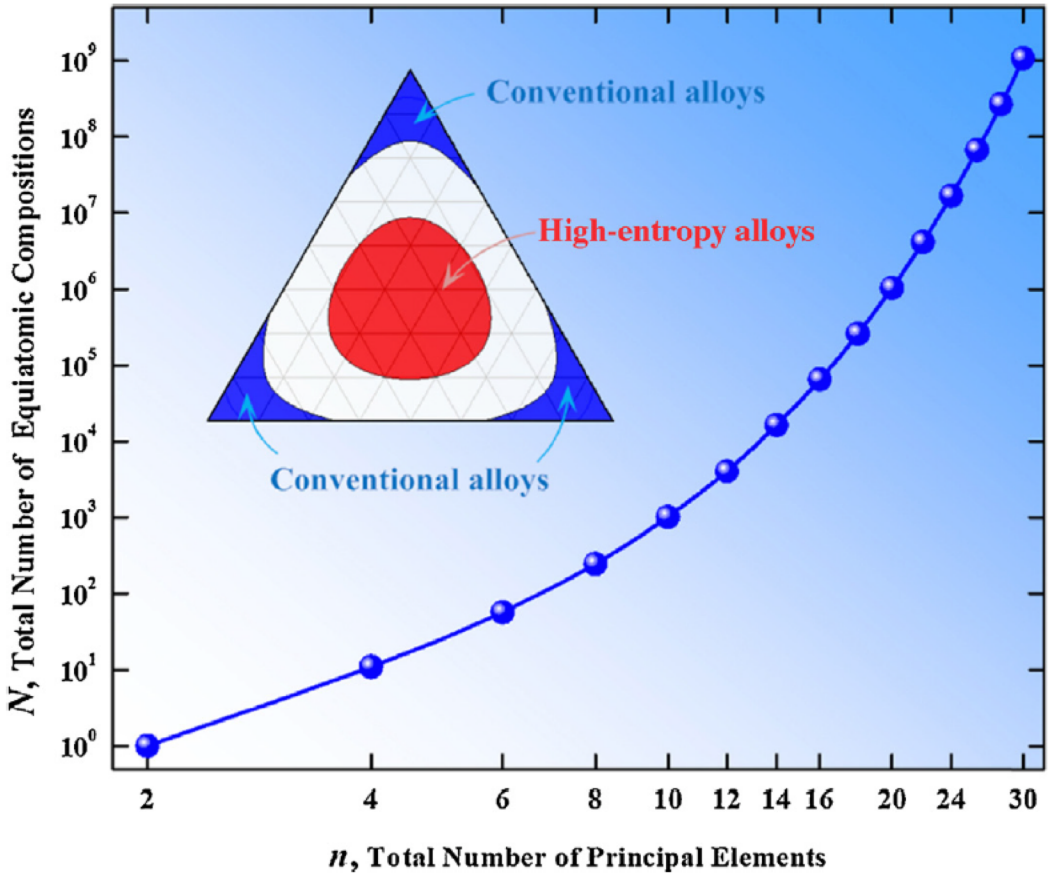
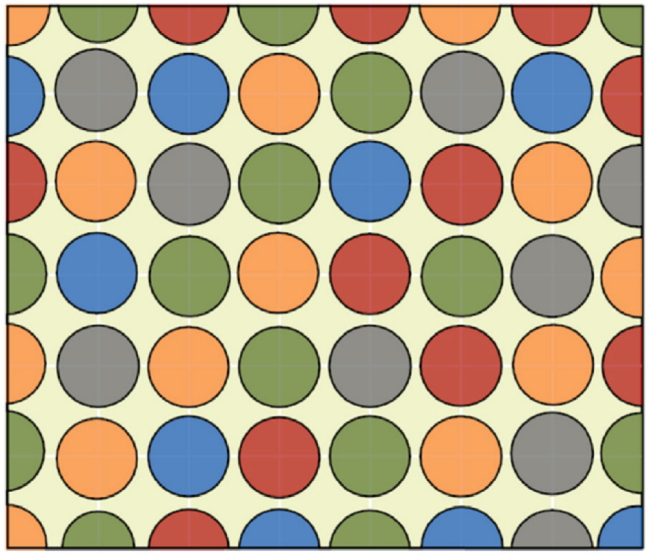


FIGURE 1

The variation in the total number of equiatomic compositions with the total number of principal elements. The inset illustrates the difference between the design of conventional alloys and high-entropy alloys on a ternary plot.



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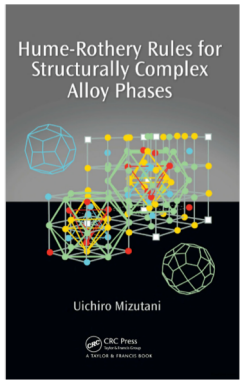
Research
Review

High-entropy alloy: challenges and prospects

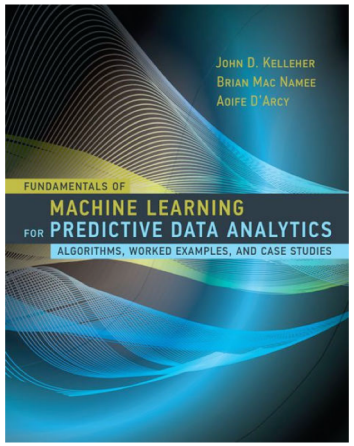
Y.F. Ye, Q. Wang, J. Lu, C.T. Liu, Y. Yang

Hume-Rothery Rules

1. The difference between the electronegativities, $\Delta\chi$, of the elements involved. The larger the $\Delta\chi$, the higher is the tendency for the atoms to unite in either liquid or solid phases. This is often called the *electrochemical effects*.
2. A tendency for atoms of elements near the ends of the short periods and B subgroups to complete their octets of electrons.
3. Size factor effects, that is, effects related to the difference in the atomic diameters of the elements.
4. A tendency for definite crystal structures to occur at characteristic numbers of electrons per unit cell, which, if all atomic sites are occupied, is equivalent to saying that similar structures occur at characteristic electrons per atom ratio **e/a** or the electron concentration.*
5. Orbital-type restrictions.

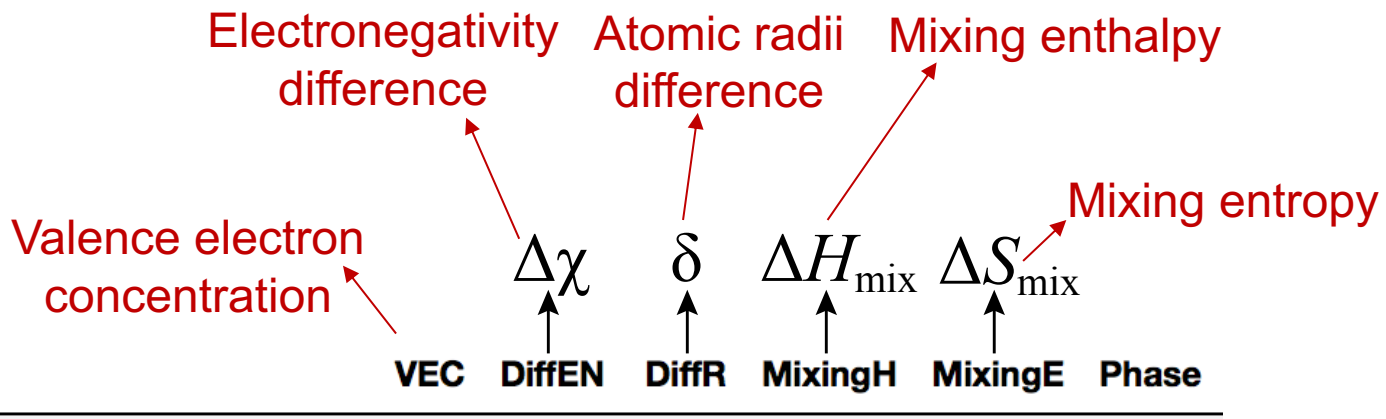


Machine Learning



Phase selection in multicomponent alloys

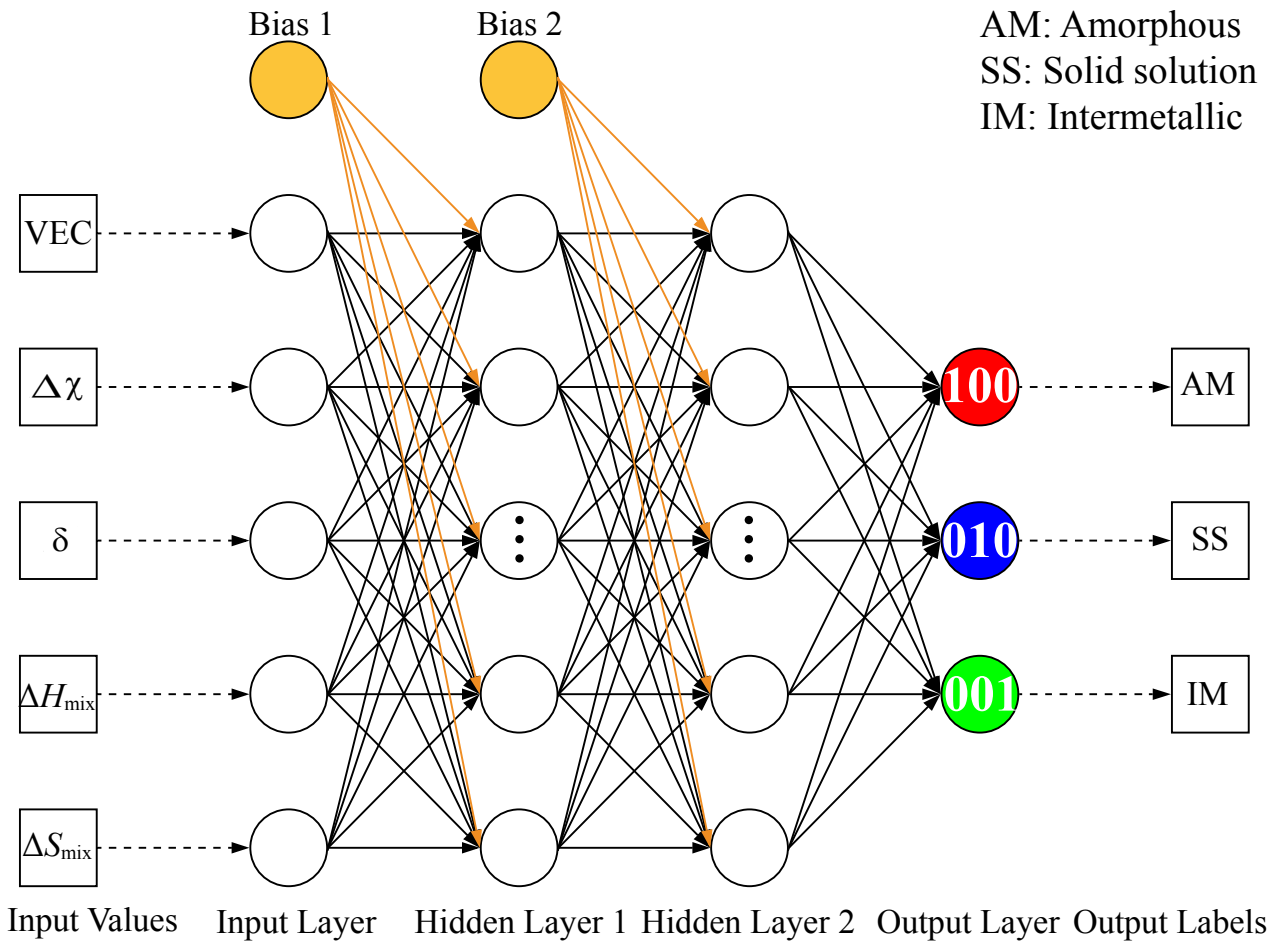
An Example of Alloy Data Set



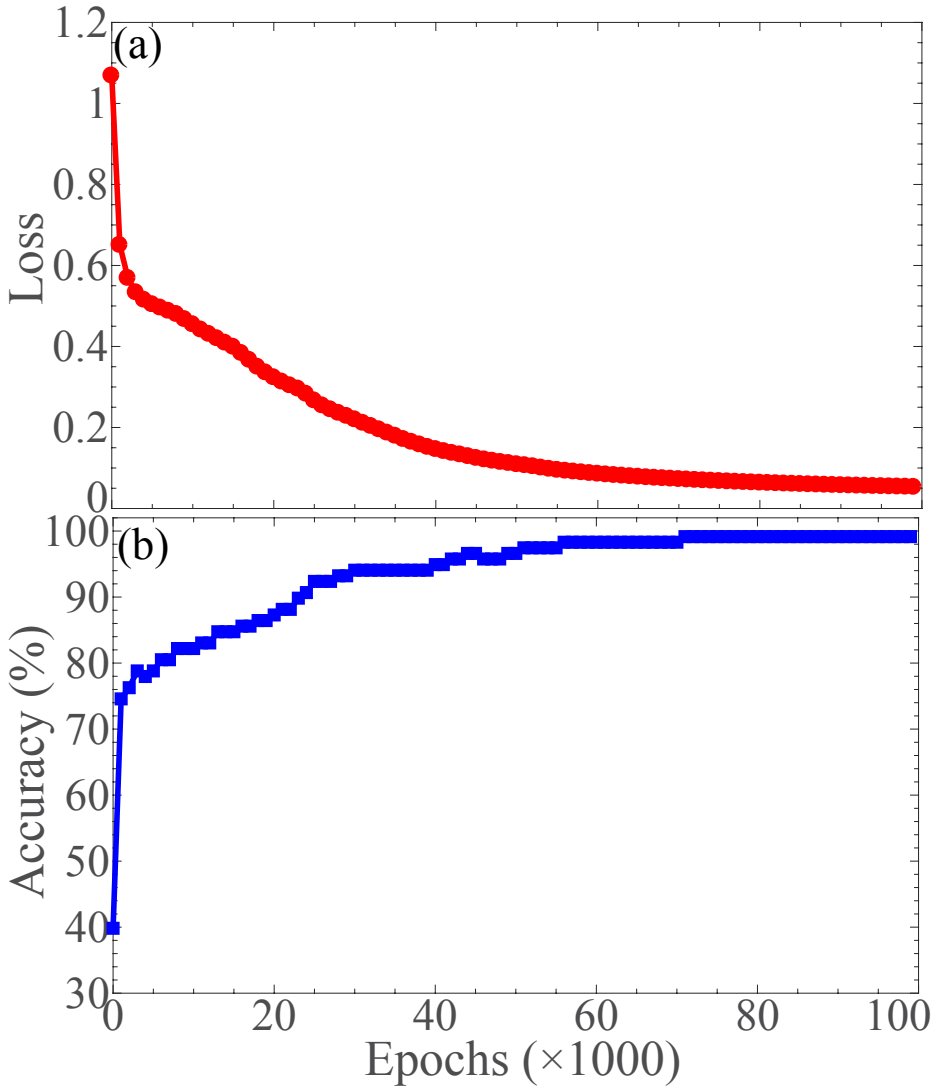
	VEC	DiffEN	DiffR	MixingH	MixingE	Phase
Cu0.5NiAlCoCrFeSi	7.00	0.12	6.35	-22.58	16.01	AM
Zr17Ta16Ti19Nb22Si26	4.38	0.20	11.08	-48.64	13.25	AM
Cu50Zr50	7.50	0.29	11.25	-23.00	5.76	AM
Ni50Nb50	7.50	0.16	6.84	-30.00	5.76	AM
PdPtCuNiP	9.20	0.16	9.29	-23.68	13.38	AM
SrCaYbMgZn	4.20	0.26	15.25	-13.12	13.38	AM

AM: Amorphous
SS: Solid solution
IM: Intermetallic

Deep-Learning Neural Network



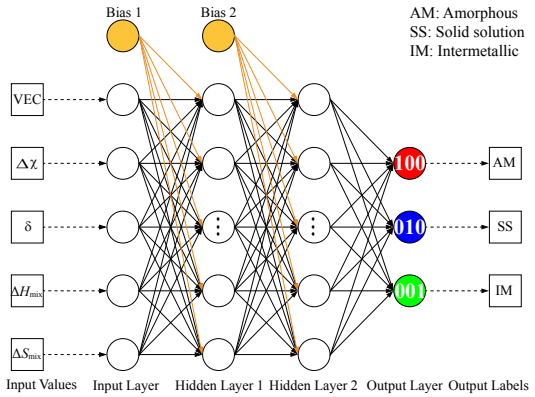
Training the Complete Data Set

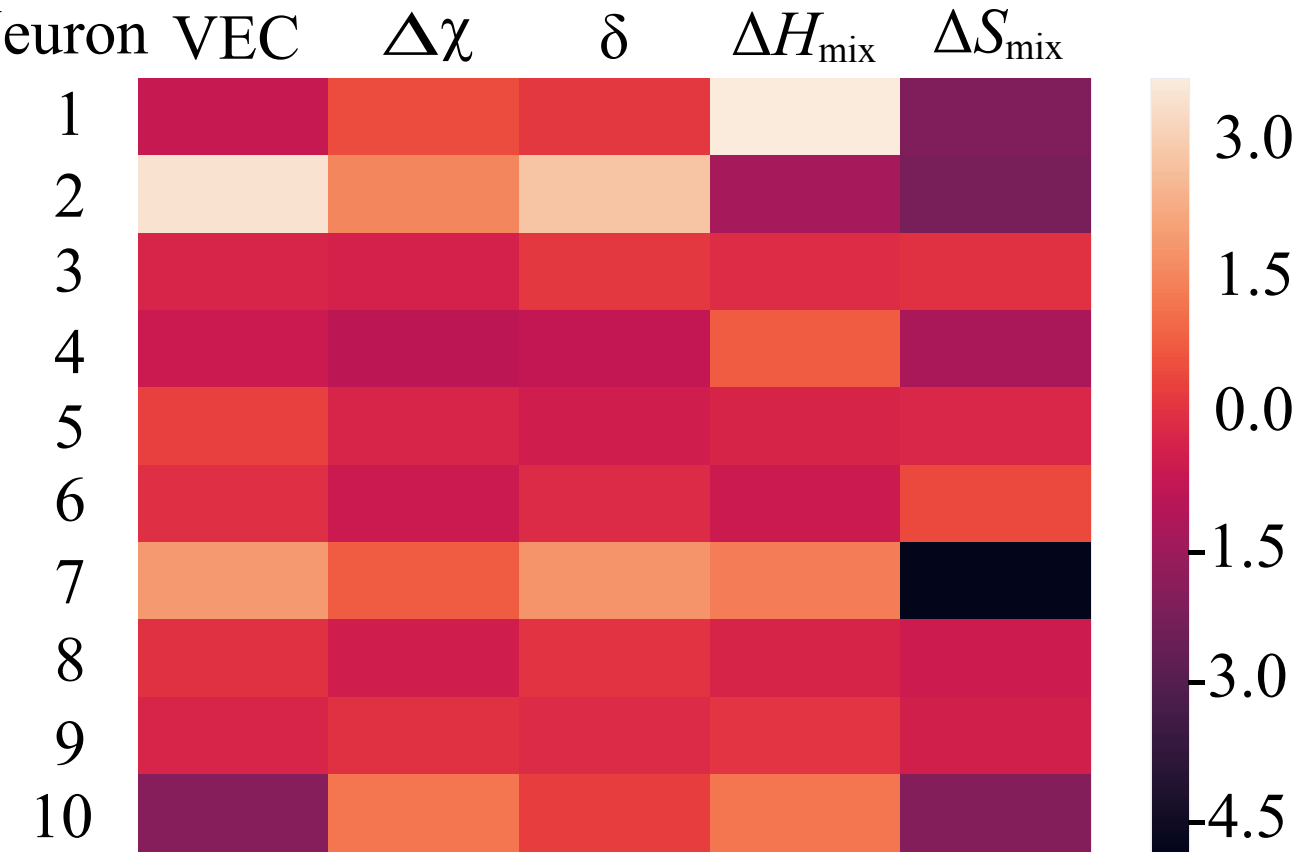


"With four parameters I can fit an elephant, and with five I can make him wiggle his trunk"

John von Neumann

Weight Matrix and Singular Value Decomposition

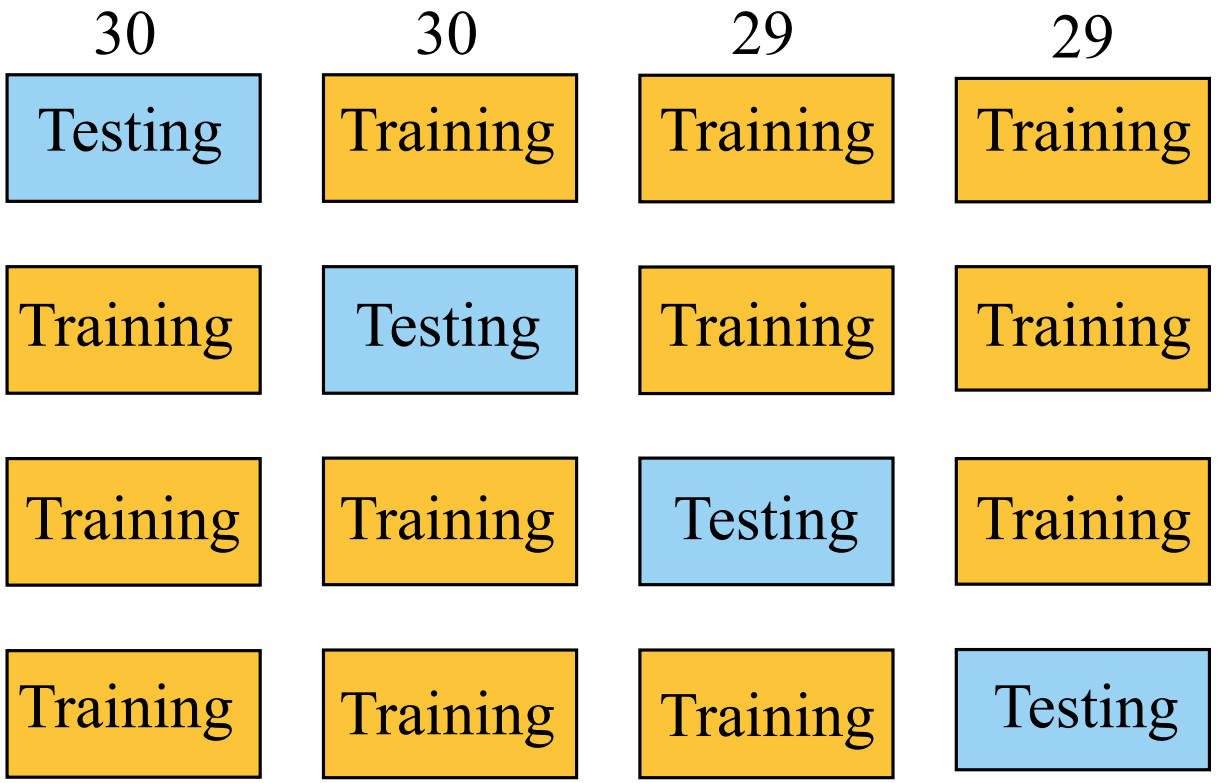




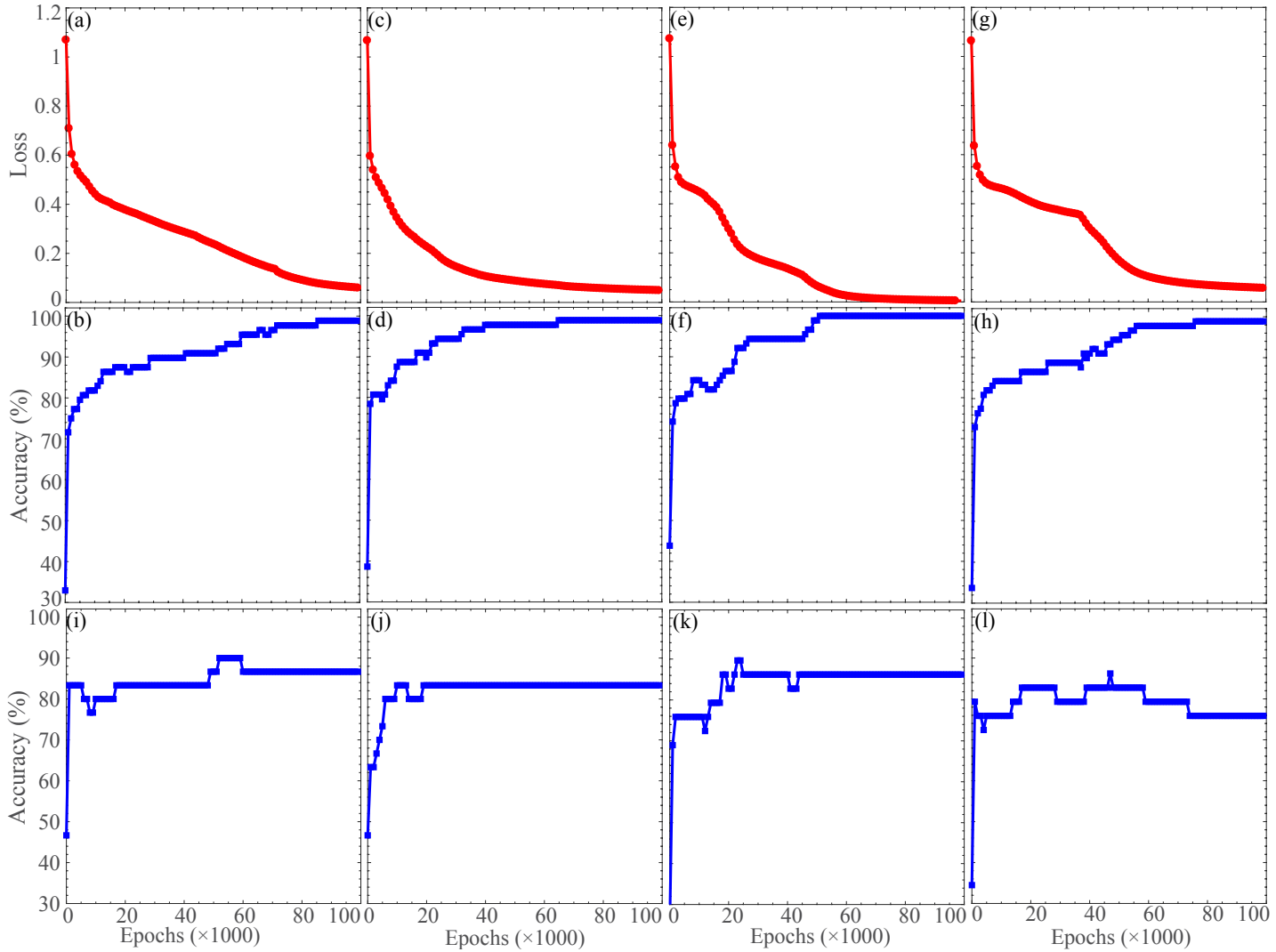
$$A = U\Sigma V^T$$

Singular values: $\mathrm{VEC} > \Delta\chi > \Delta H_{\mathrm{mix}} > \delta > \Delta S_{\mathrm{mix}}$

Cross-Validation



Cross-Validation: Training and Testing



Ongoing Work: Applying ML to High Entropy Alloys

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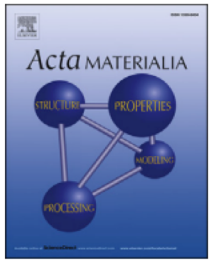

By invitation only: overview article

A critical review of high entropy alloys and related concepts

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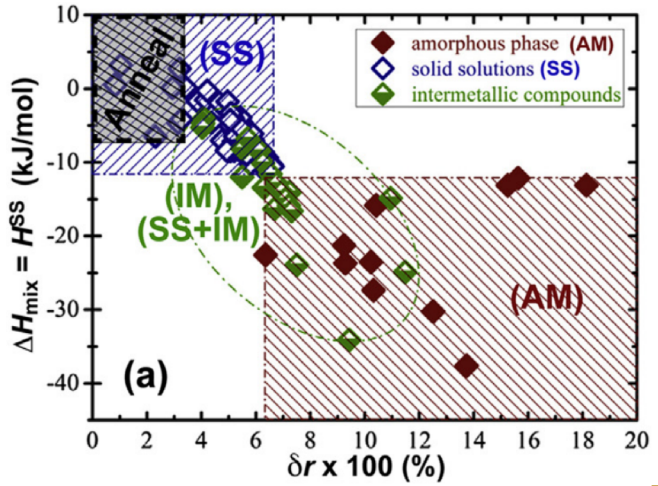

Acknowledgements

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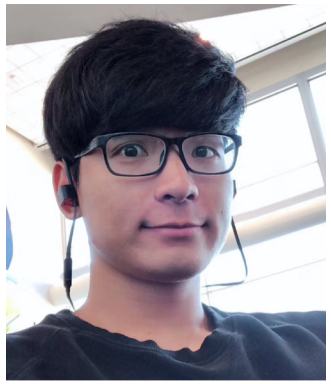

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