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Design and development of equi-atomic refractory High Entropy Alloys for use in radiation environments

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Changing the World's Energy Future

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Design and development of equi-atomic refractory High Entropy Alloys for use in radiation environments

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Background

Development of new structural materials that can withstand the extreme environments of nuclear reactors where the materials are exposed to high dose rate of ~ 30 – 200 dpa, high temperatures of the order of 500 -1000 ºC and tens of years of operation is vital for exploiting the "smallest carbon footprint energy source" to its fullest, in order to deal with the energy crisis worldwide.

Recently, HEAs have shown superior irradiation properties over conventional alloys like higher resistance to defect formation, lower void swelling, limited irradiation hardening and higher microstructural stability under irradiation, making them potential structural material candidates for reactors.

Proper characterization and testing of these materials are essential before they can replace the conventional alloys.

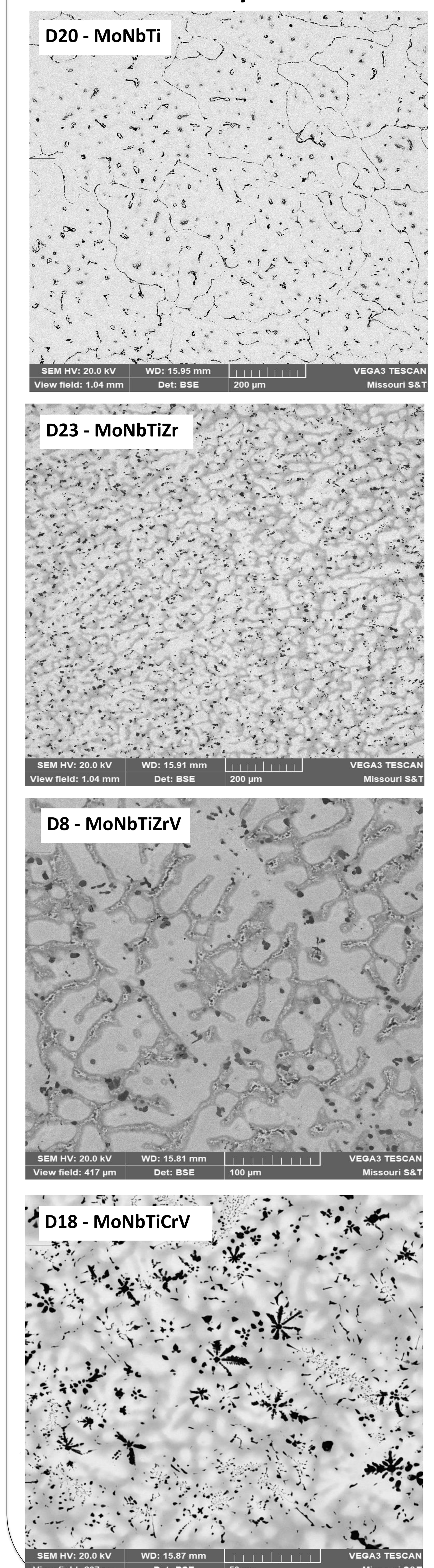
Methodology

The nature of solid solution that four equi-atomic HEA systems composed of low neutron cross section refractory elements can form was predicted by calculating empirical thermodynamic parameters. Phase formation in them was predicted by calculation of Equilibrium and Non equilibrium diagrams using the CALPHAD approach.

Vacuum arc melting was used to fabricate the materials from powder raw material compacted to briquette form. Xray diffraction (XRD) was utilized to identify the structures of the phases in the as cast alloys. The microstructures were analyzed under the Scanning Electron Microscope (SEM) and the chemistry of the phases were obtained by Energy Dispersive Spectroscopy (EDS). Phase evaluation at the high service temperature range (500 – 1000 ºC) of Gen IV rectors were done using quenching dilatometry technique.

Calculations and Results

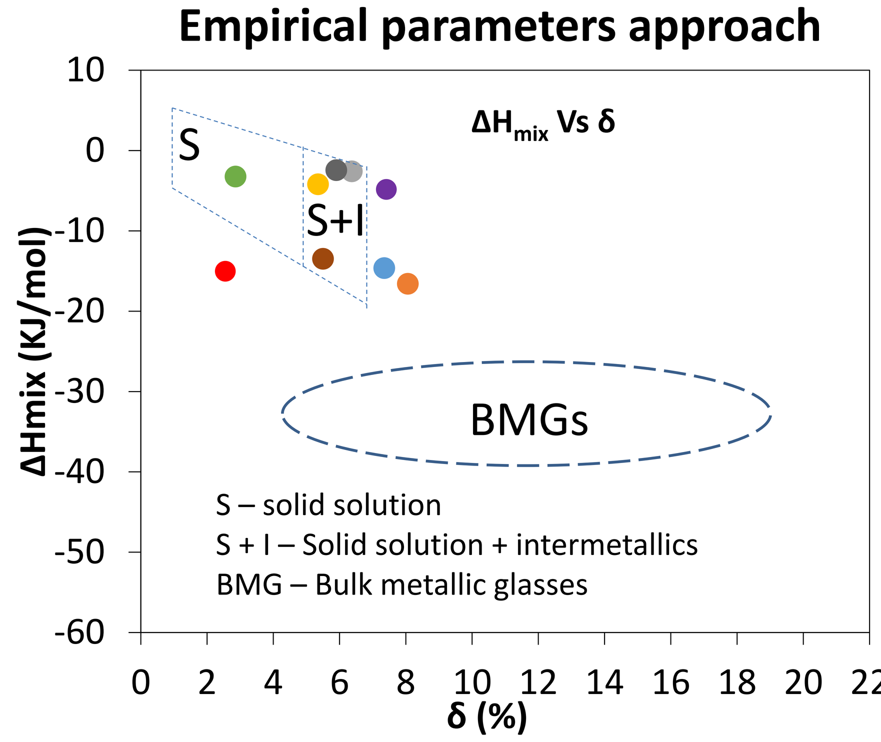
SEM analysis

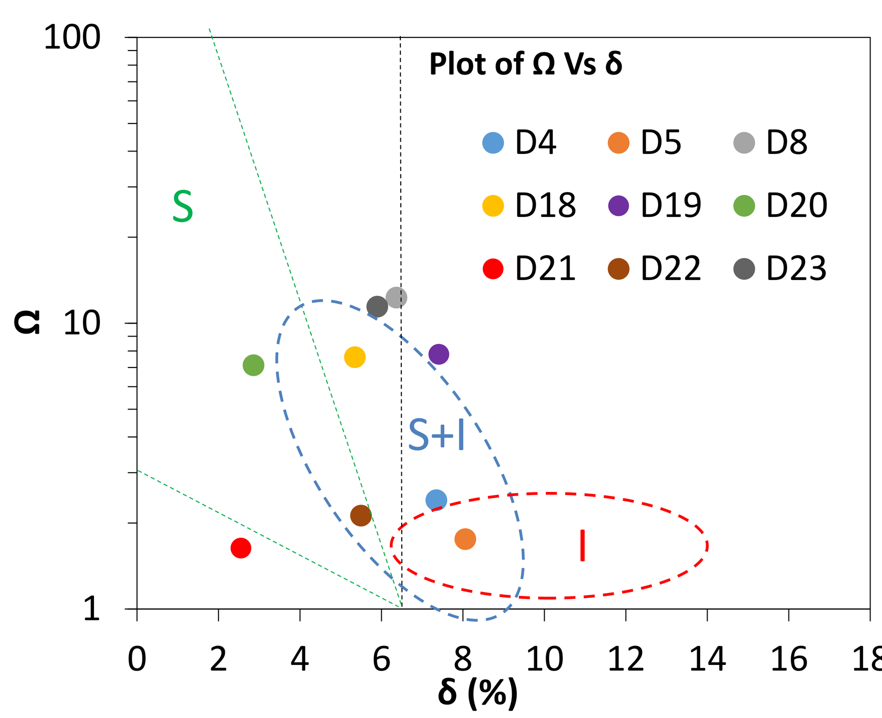


Elemental selection

Elements	r [Å]	T_m [K]	ρ [g/cm³]	σ_A [barns]
Ti	1.462	1941	4.51	6.09
V	1.34	2183	6.12	5.08
Cr	1.249	2180	7.19	3.05
Zr	1.6	2128	6.51	0.185
Nb	1.429	2750	8.58	1.15
Mo	1.363	2896	10.23	2.48

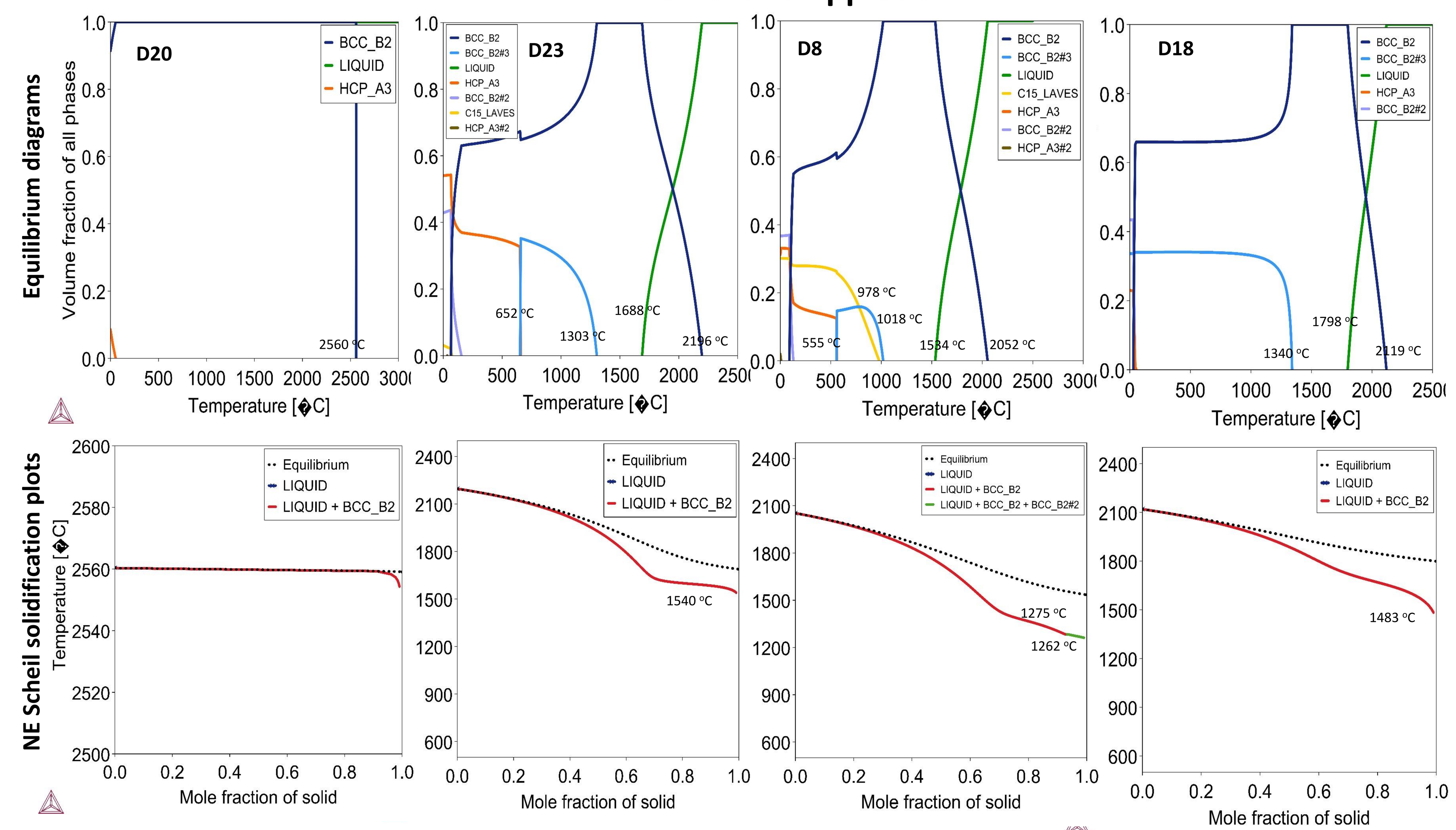
Empirical parameters approach



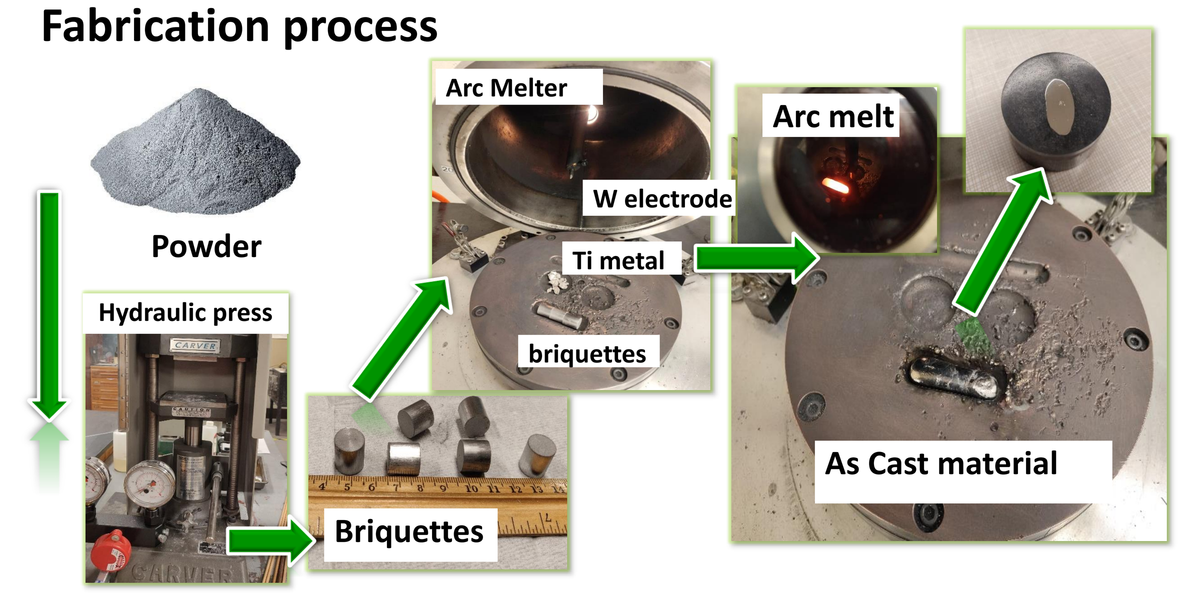


EDS results		Nb	Mo	Ti	Zr	V	Cr
D20	D	38.05	43.02	18.75	D – dendrites		
	I/black	6.95	1.43	91.62	I – Interdendrities		
D23	D	30.93	31.54	29.06	8.47		
	I	16.56	16.23	29.30	37.91		
	Black	5.06	0.00	20.21	74.73		
D8	D	26.71	30.11	17.74	5.82	19.61	
	I_{dark}	16.60	16.67	23.76	17.09	26.28	
	I_{light}	4.61	1.78	38.14	50.24	5.23	
	Black	3.72	0.00	16.40	79.21	0.67	
D18	D_{grey}	21.29	29.34	16.04		19.54	14.00
	D_{light}	17.70	13.23	21.00		21.51	26.56
	Black rosettes	2.12	2.08	81.20		4.35	10.25

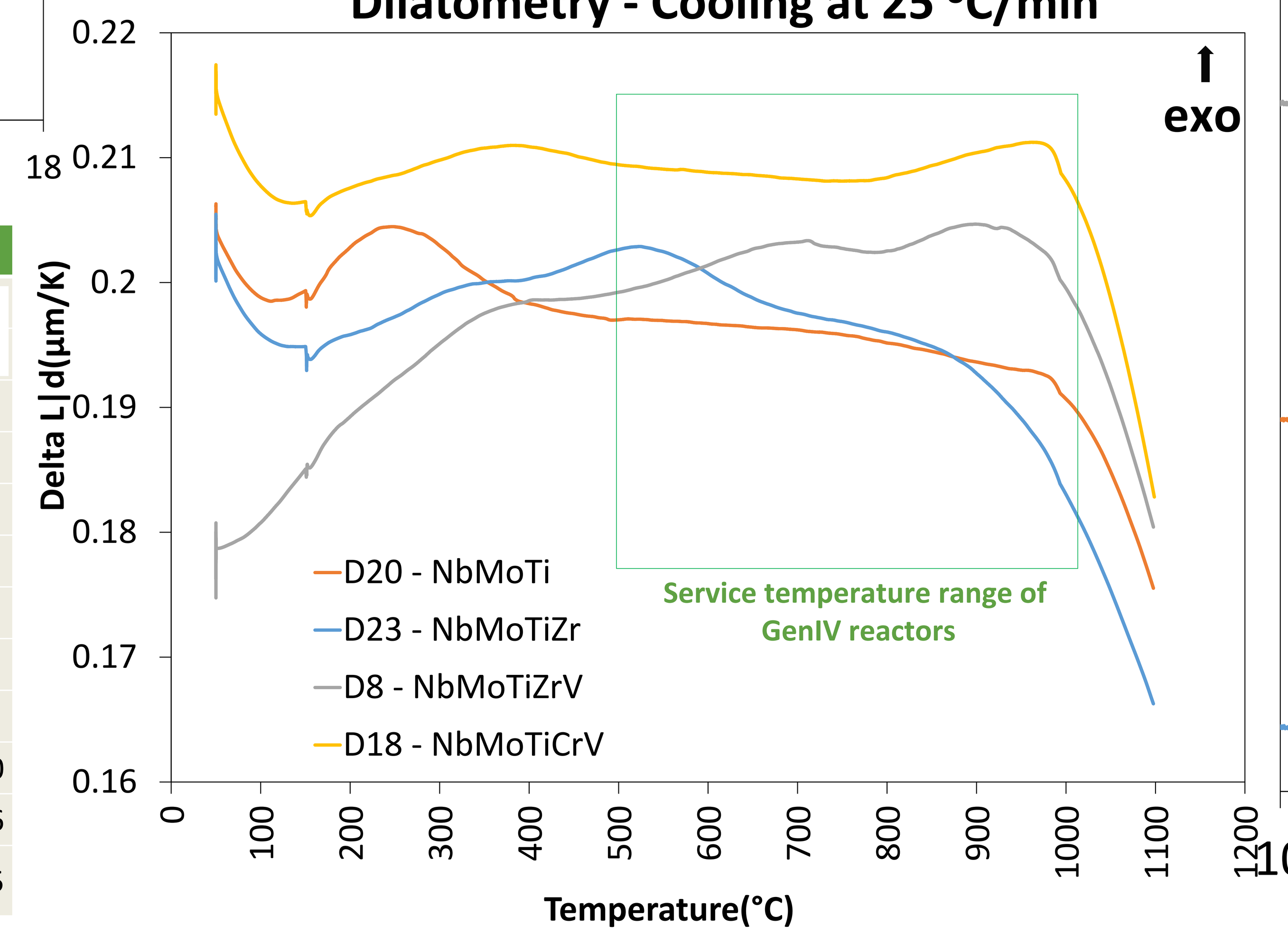
CALPHAD approach



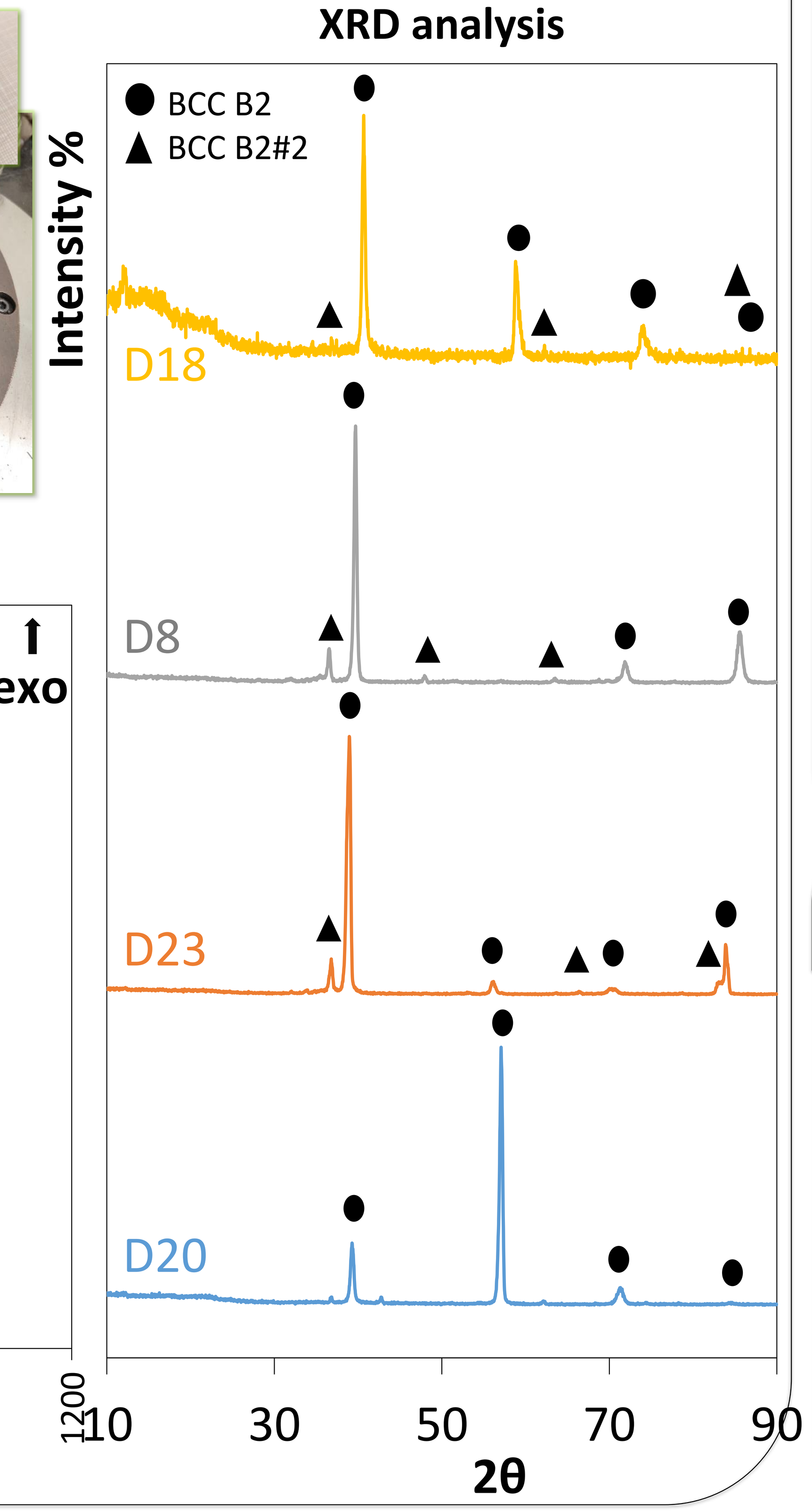
Fabrication process



Dilatometry - Cooling at 25 ºC/min



XRD analysis



Conclusions

- Four equi-atomic refractory high entropy alloys, D20, D23, D8 and D18 were successfully designed using empirical and Calphad approach.
- XRD results validated the Empirical and Calphad predictions and SEM analysis for chemistry and microstructure reinforced the existence of multiple phases in the systems.
- High temperature phase evaluation using dilatometry showed the phases that would form at the operational temperature range of Gen IV reactors.

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Future Works

- More high temperature tests on the system.
- Mechanical property and Air oxidation testing of the materials
- Irradiation and post irradiation characterization and property evaluation.
- Compositional modifications