



20th DISCUSSION MEETING ON THERMODYNAMICS OF ALLOYS
20 - 24 September 2026
BLLED - SLOVENIA

Phase relations in the $\text{ZrO}_2\text{-Y}_2\text{O}_3\text{-Dy}_2\text{O}_3$ system

Danilo Alencar de Abreu, Maren Lepple



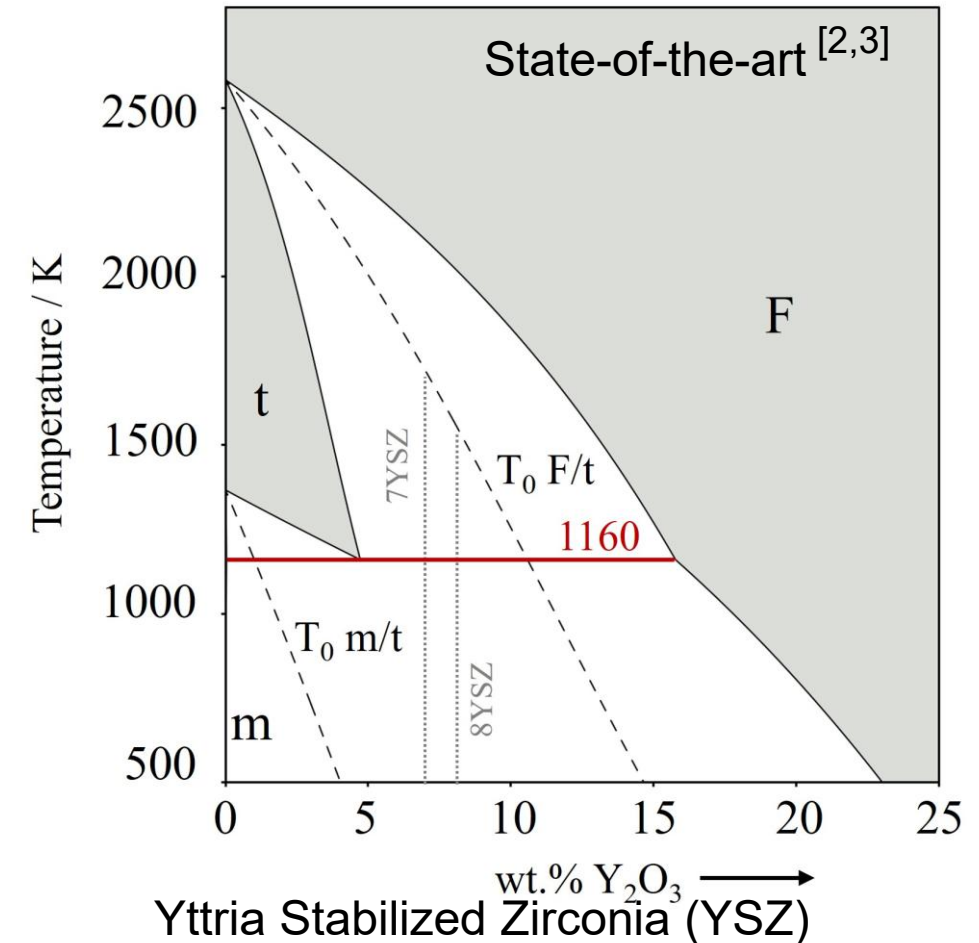
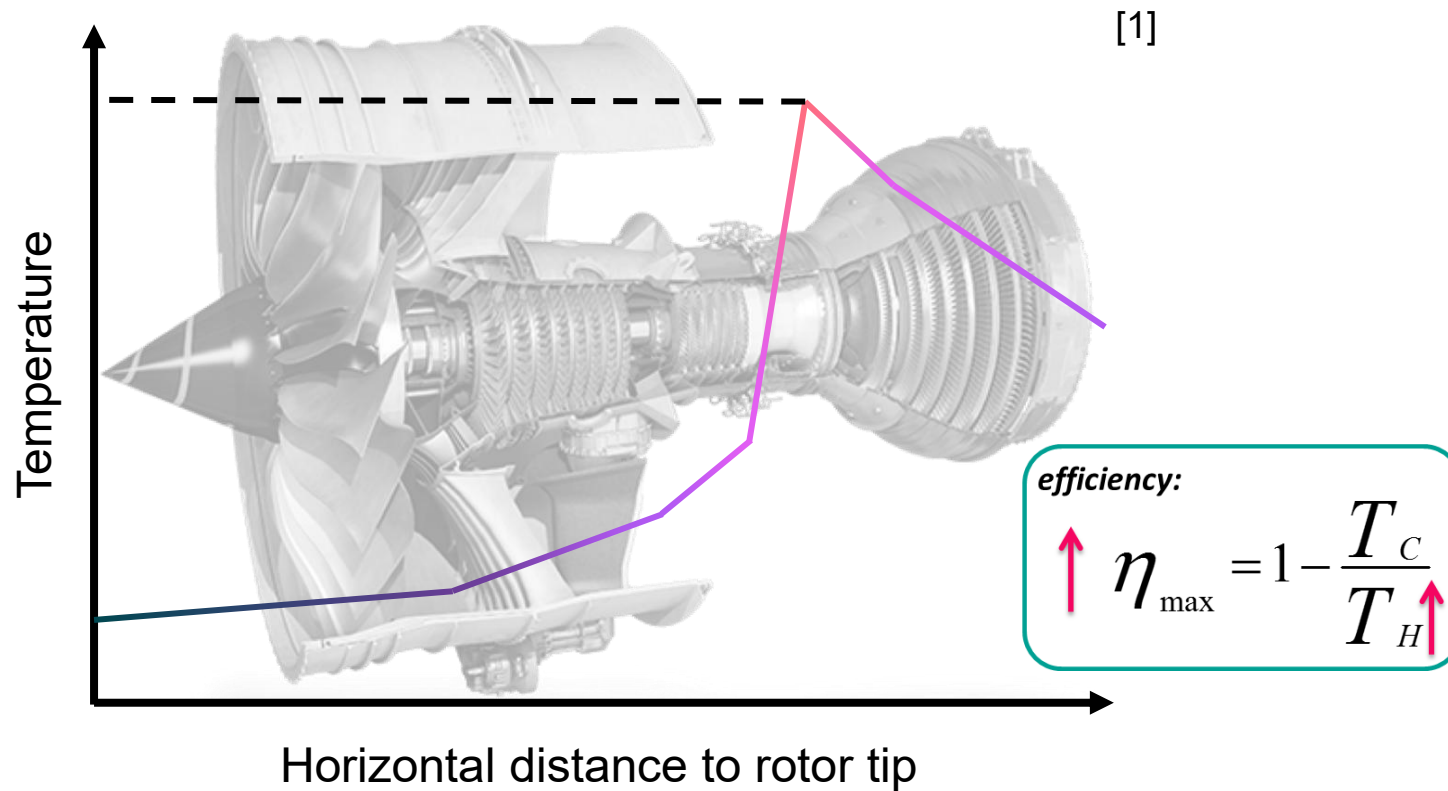
Federal Ministry
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TOFA 2026 – Bled, Slovenia

24.09.2026

Thermal Barrier Coatings (TBCs)

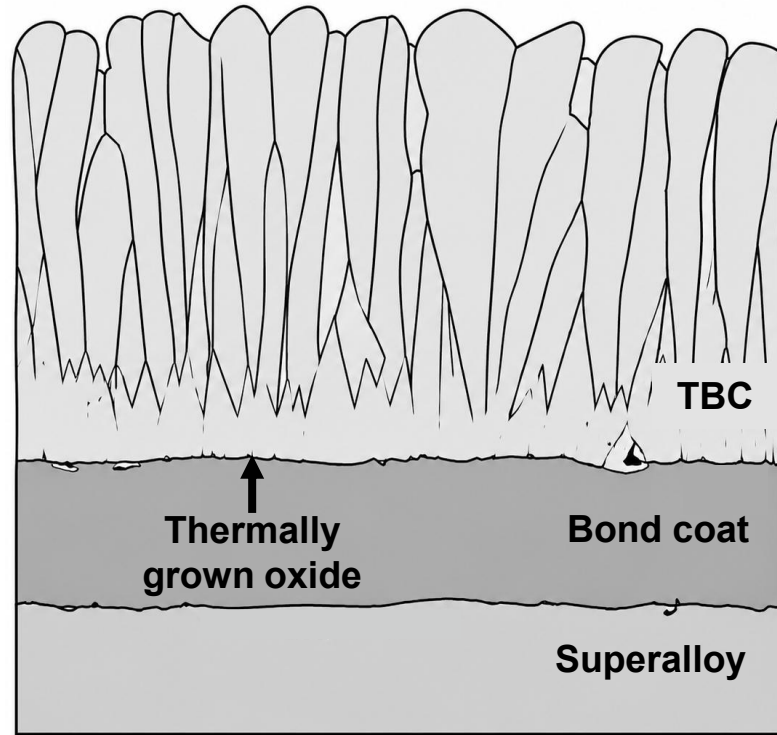


Enhance the efficiency ➡ reduction of emissions

[1] M. Bogdan, I. Peter, *Metals* **2024**, 14, 575.

[2] O. Fabrichnaya et al., *J. Phase. Equilib. Diffus.* **2011**, 32, 2-16.

[3] A. Habermann et al., *Solid State Sciences* **2026**, 108482.



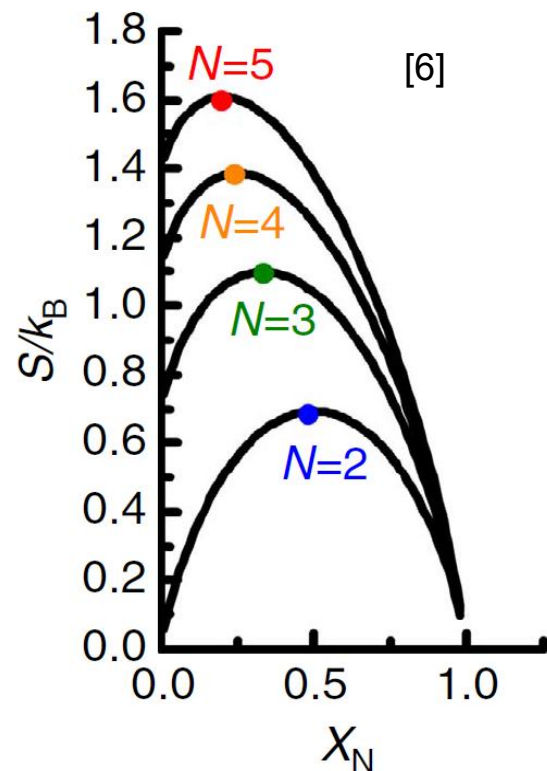
[4]

- ▶ High melting point
- ▶ Sluggish diffusion
- ▶ Low thermal conductivity
- ▶ No phase transformations (rt $\rightleftharpoons$ ht)
- ▶ Matching coefficients of thermal expansion with substrate and bond coat
- ▶ Sufficient mechanical properties
- ▶ Chemical resistance

[5]

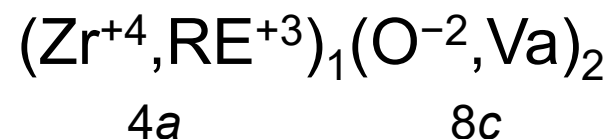
[4] A. Anupam, S. Joshi, *J. Eur. Ceram. Soc.* **2025**, 46(14), 118499.

[5] J. Song et al., *Coatings* **2023**, 13, 343.

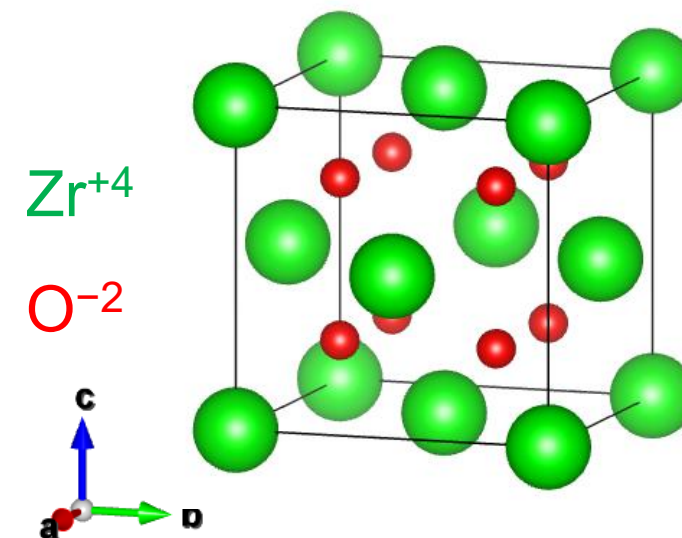


► Multi-component rare-earth zirconates $\text{RE}_2\text{Zr}_2\text{O}_7$ with 5 or more cations (pyrochlore or defect-fluorite structure) [7,8]

Fluorite



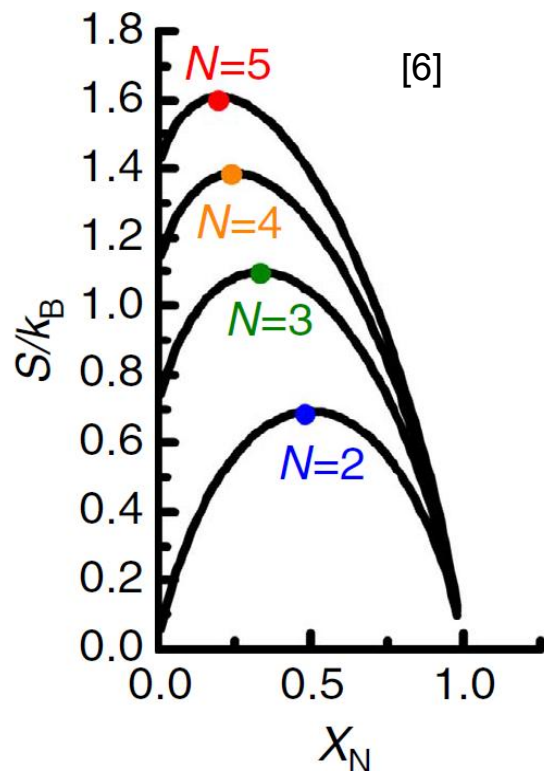
$$\text{conf. } S = -R \sum_{i=1}^N x_i \ln(x_i) > 1.5 R$$



[6] C. M. Rost *et al.*, *Nat. Commun.* **2015**, 6, 8485.

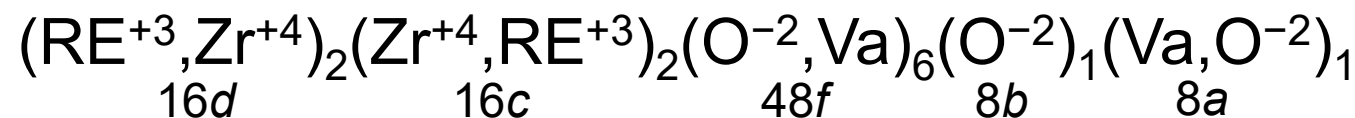
[7] A. Sarkar *et al.*, *Adv. Mater.* **2019**, 31, 1806236.

[8] L. Luo *et al.*, *J. Eur. Ceram. Soc.* **2024**, 44, 2250-2559.



► Multi-component rare-earth zirconates $\text{RE}_2\text{Zr}_2\text{O}_7$ with 5 or more cations (pyrochlore or defect-fluorite structure) [7,8]

Pyrochlore



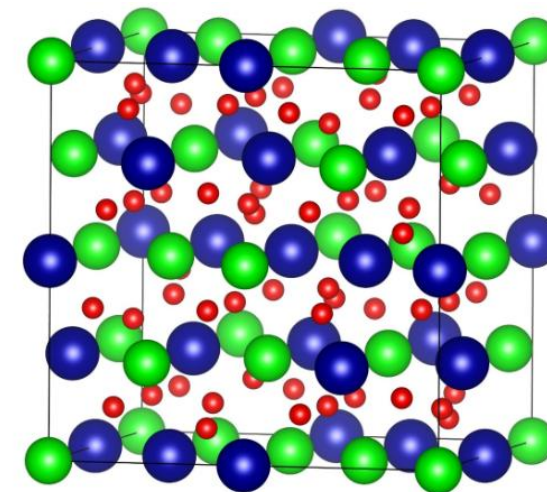
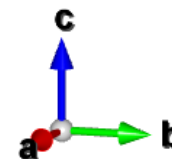
$$\text{conf. } S = -R \sum_{i=1}^N x_i \ln(x_i) > 1.5 R$$



RE^{+3}

Zr^{+4}

O^{-2}

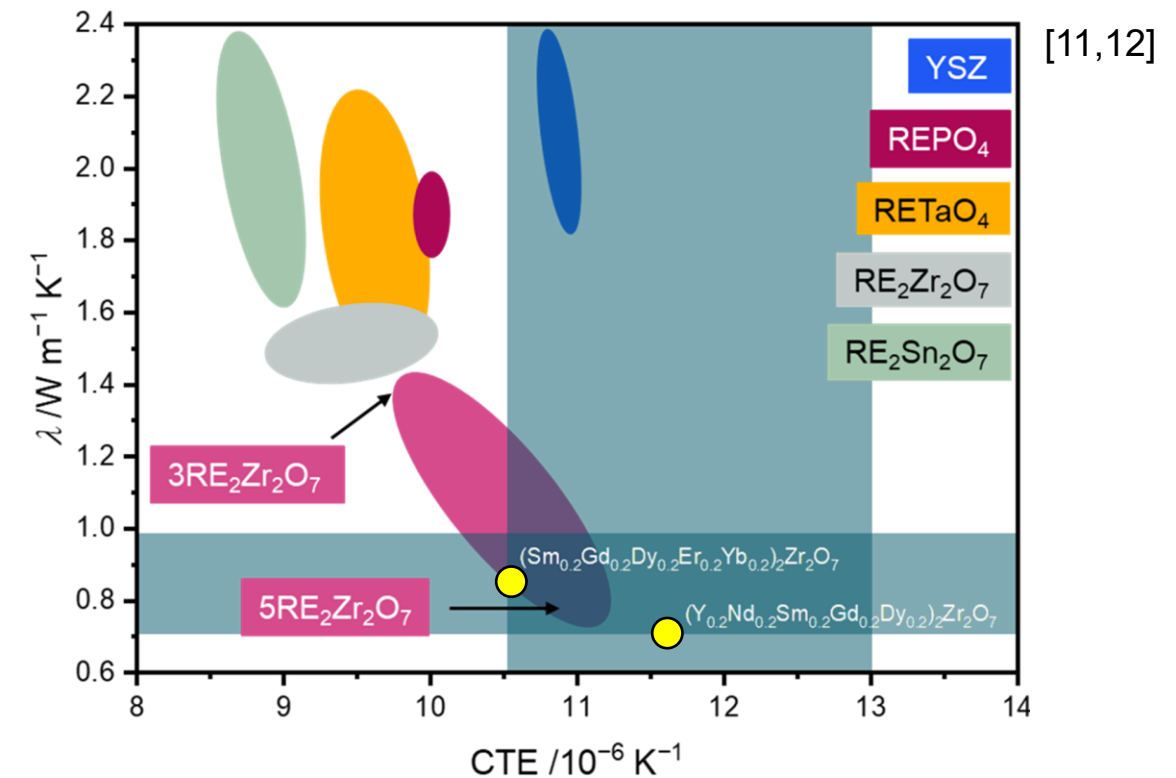
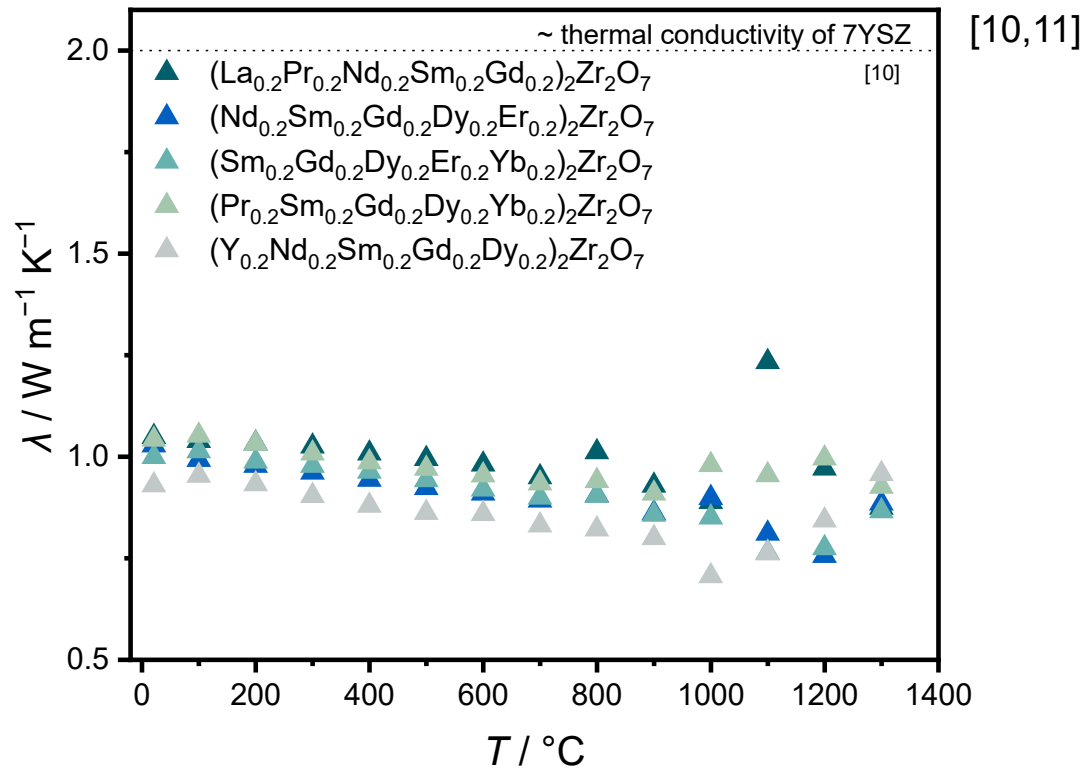


[6] C. M. Rost *et al.*, *Nat. Commun.* **2015**, 6, 8485.

[7] A. Sarkar *et al.*, *Adv. Mater.* **2019**, 31, 1806236.

[8] L. Luo *et al.*, *J. Eur. Ceram. Soc.* **2024**, 44, 2250-2559.

► Promising composition: (Dy_{0.2}Gd_{0.2}Nd_{0.2}Sm_{0.2}Y_{0.2})₂Zr₂O₇ [9]



[9] P. Hutterer *et al.*, *J. Am. Ceram. Soc.* **2023**, 106, 1547.

[10] E. Bakan *et al.*, *Elsevier series on advanced ceramic materials*, Elsevier, **2020**.

[11] P. Hutterer *et al.*, *Dissertation* **2025**.

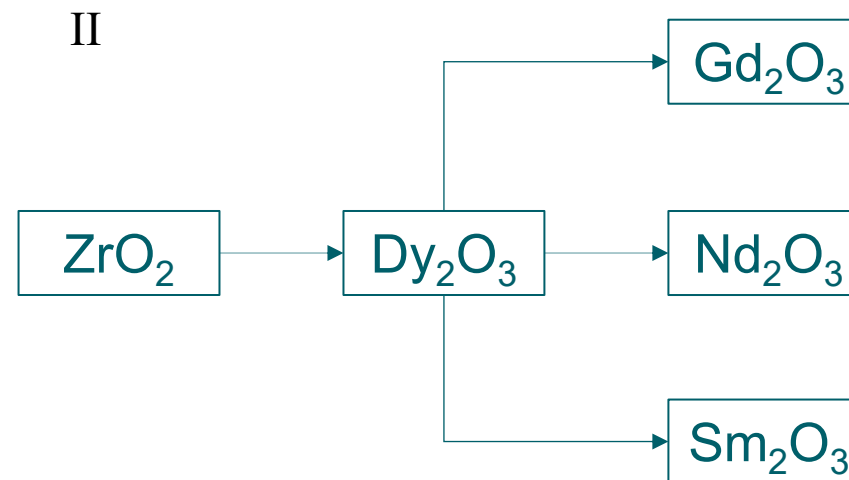
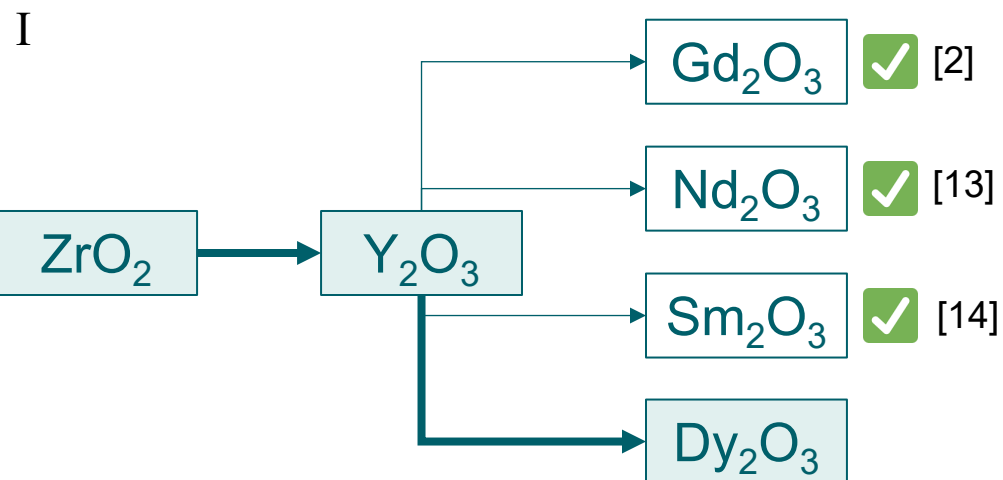
[12] K. Ren *et al.*, *Scripta Materialia* **2020**, 178, 382.

- ▶ Multicomponent system: $\text{ZrO}_2\text{-Dy}_2\text{O}_3\text{-Gd}_2\text{O}_3\text{-Nd}_2\text{O}_3\text{-Sm}_2\text{O}_3\text{-Y}_2\text{O}_3$
- ▶ Development of a thermodynamic database using the CALPHAD method

- ▷ Microstructural changes
- ▷ Definition of suitable compositions
- ▷ Processing conditions

Thermodynamic models

- ▶ Two-sublattice partially ionic liquid model
 - ▷ Liquid
- ▶ Compound Energy Formalism (CEF)
 - ▷ ZrO_2 -based phases
 - ▷ RE_2O_3 -based phases
- ▶ Stoichiometric model
 - ▷ $\delta\text{-Zr}_3\text{Y}_4\text{O}_{12}$



III 3 subsystems

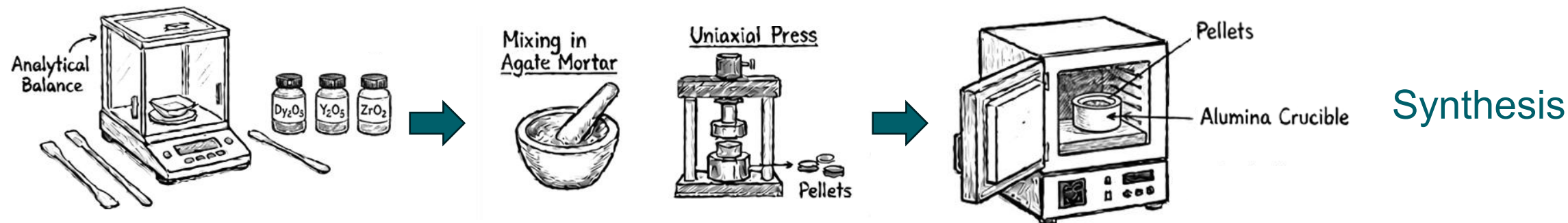


RE = Gd, Nd, Sm

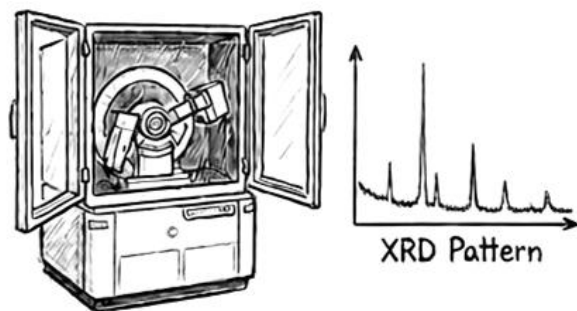
Ideal mixing in solid and liquid phases



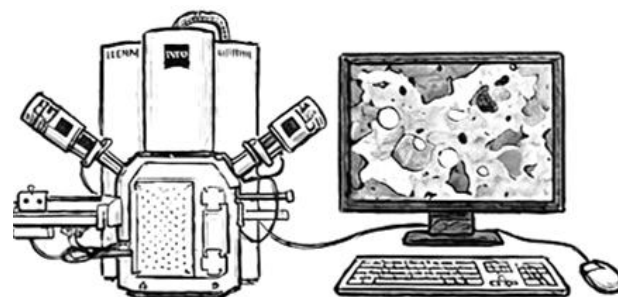
RE = Dy, Gd, Nd, Sm



Microstructural analysis

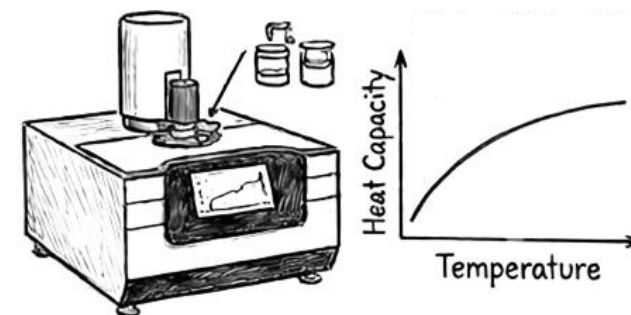


- ▷ Panalytical Empyrean
- ▷ AntonPaar XRDynamic 500



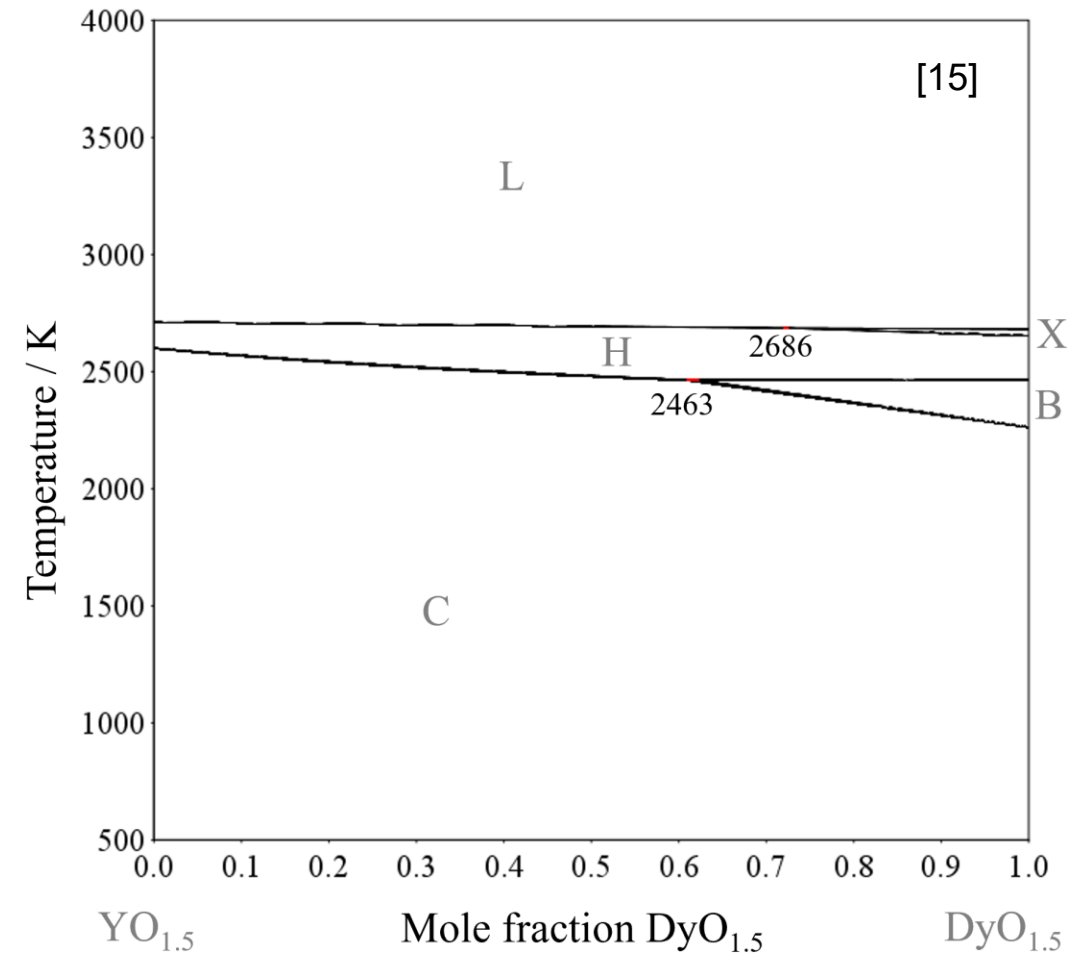
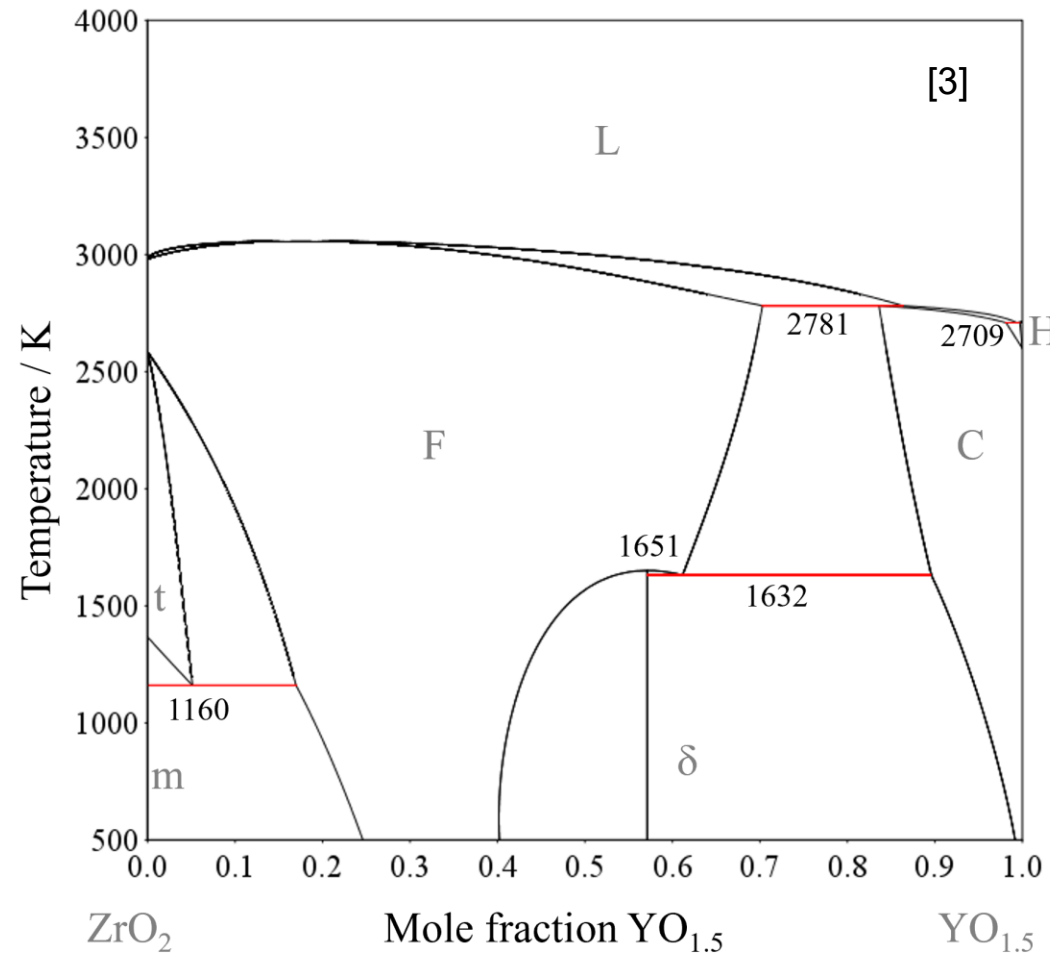
- ▷ Polishing + Carbon coating
- ▷ Zeiss Gemini 3 SEM 560
- ▷ BSE, SE, EDX

Thermal analysis



- ▷ Netzsch DSC Caliris 300
- ▷ Netzsch STA 449 Jupiter

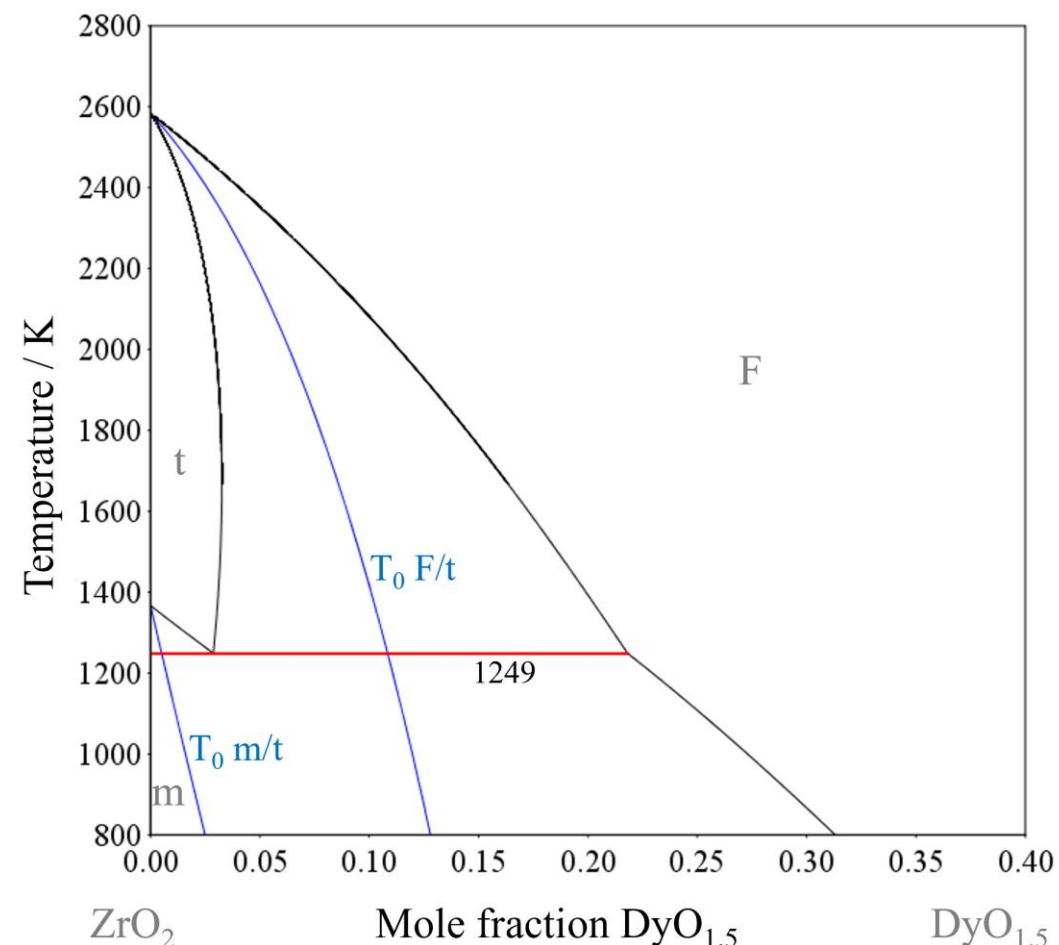
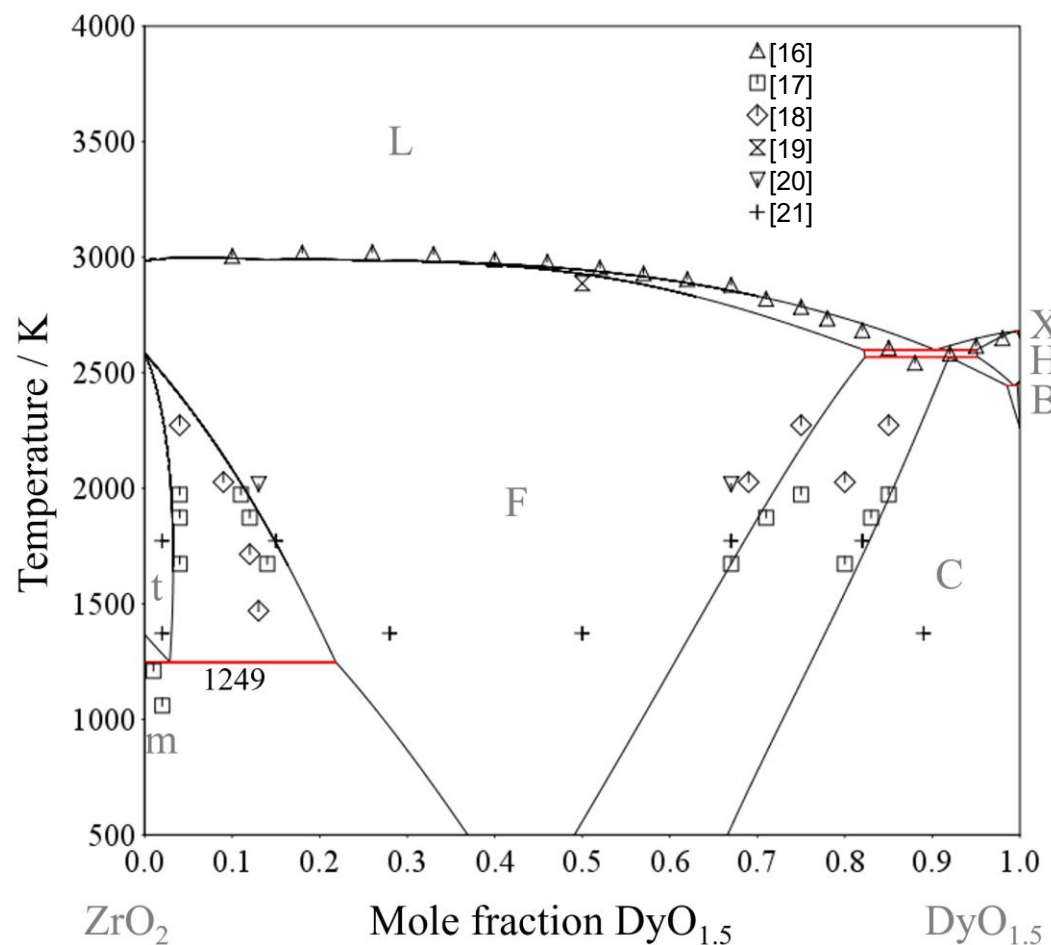
ZrO₂-Y₂O₃ and Y₂O₃-Dy₂O₃ systems



[3] A. Habermann et al., *Solid State Sciences* **2026**, 108482.

[15] M. Zinkevich, *Prog. Mater. Sci.* **2007**, 52, 597-647.

The $\text{ZrO}_2\text{-Dy}_2\text{O}_3$ system



[16] A. Rouanet, *Rev. Int. Hautes Temp. Réfract.* **1971**, 8, 161-180.

[17] C. Wang et al., *Int. J. Mater. Res.* **2007**, 98, 91-98.

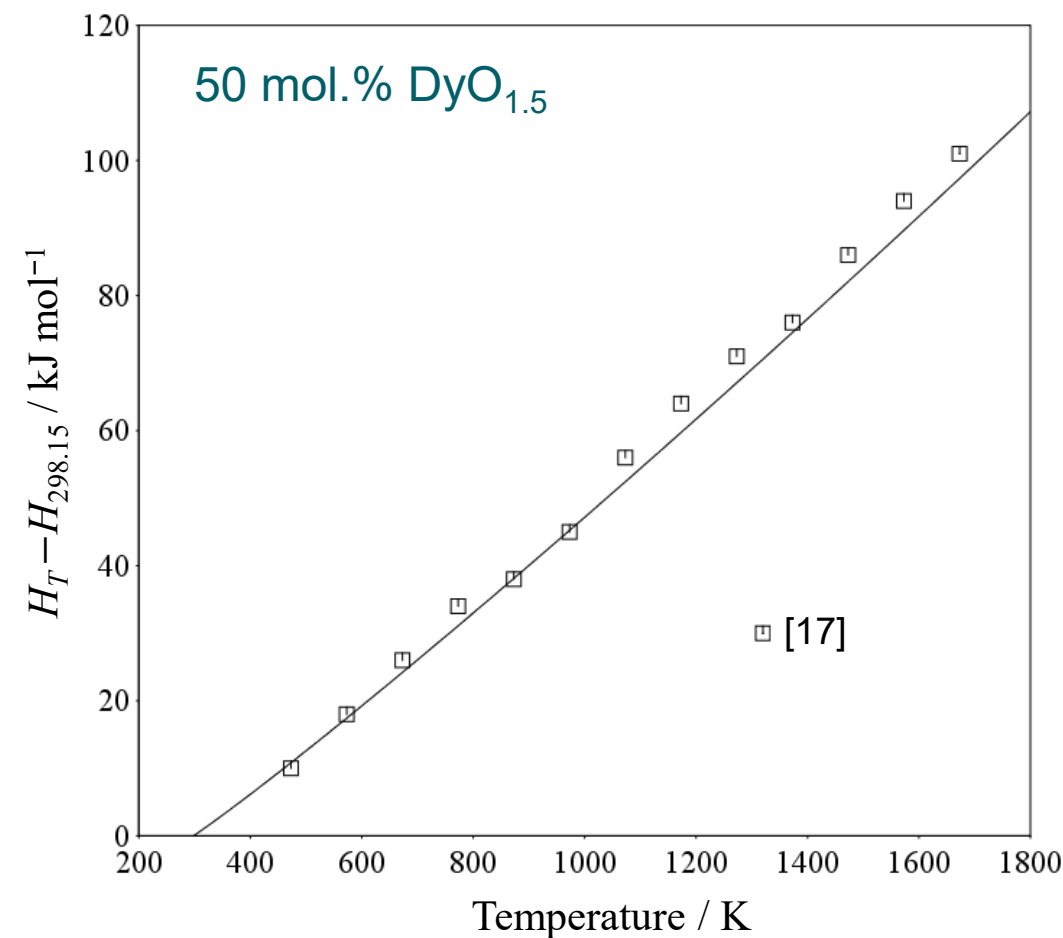
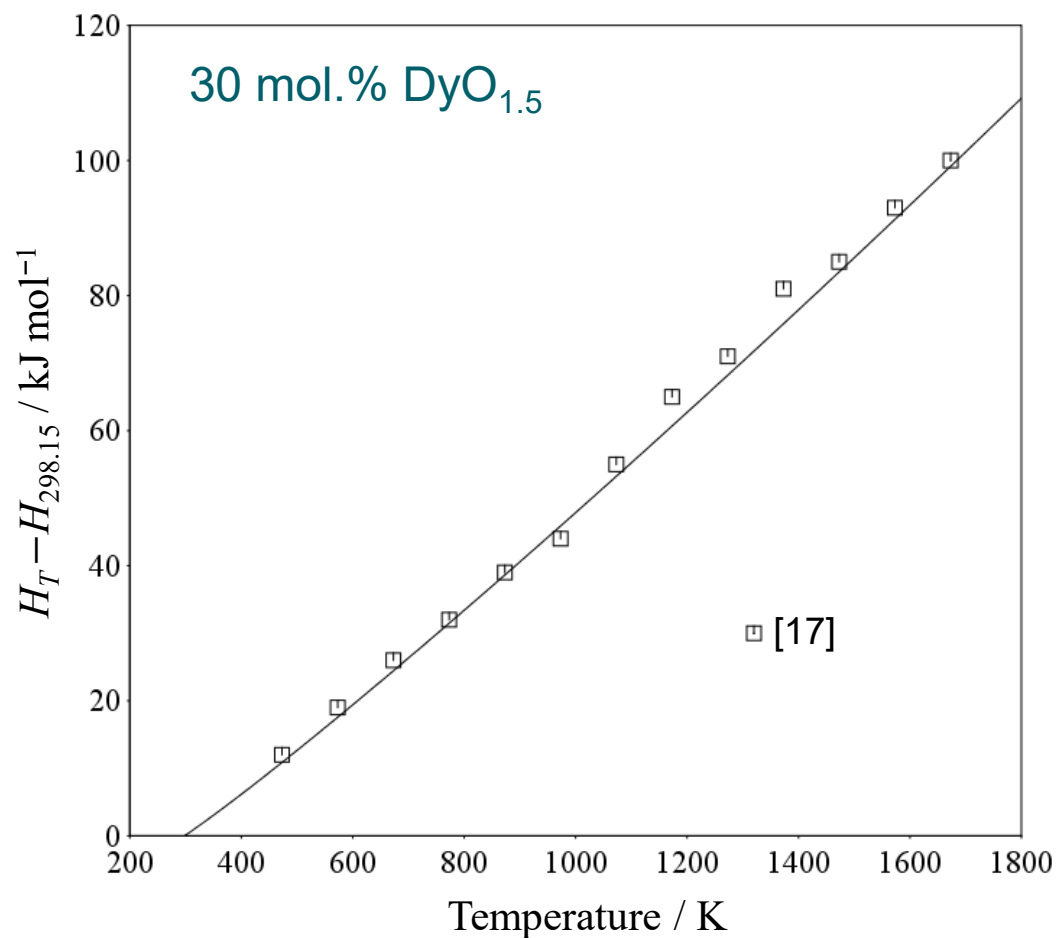
[18] C. Pascual, P. Duran, *J. Mat. Sci.* **1980**, 15, 1701-1708.

[19] E. Zoz et al., *Rus. J. Inorg. Chem.* **1982**, 8, 54-56.

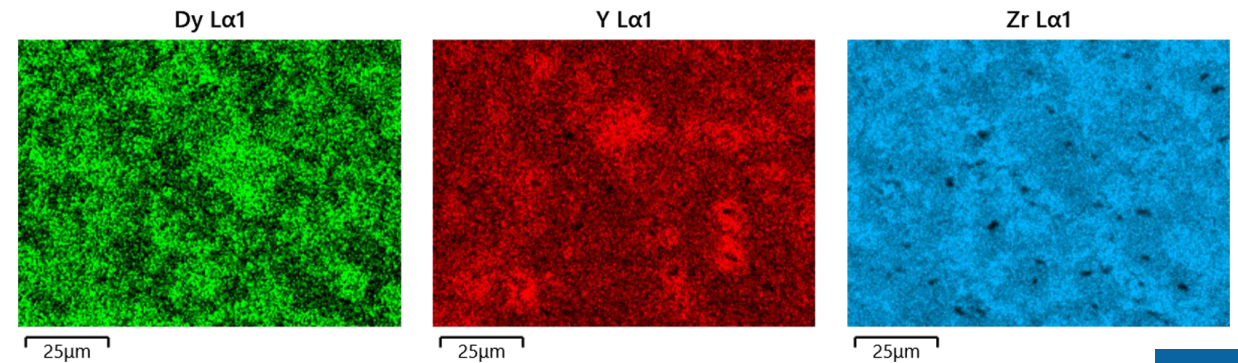
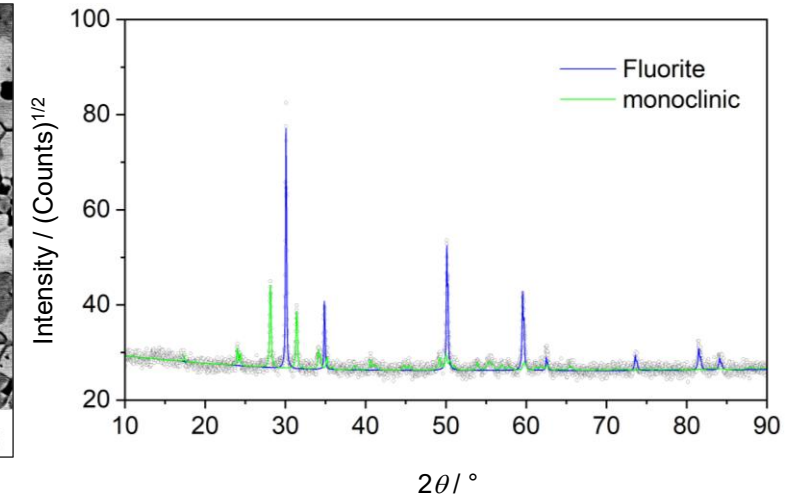
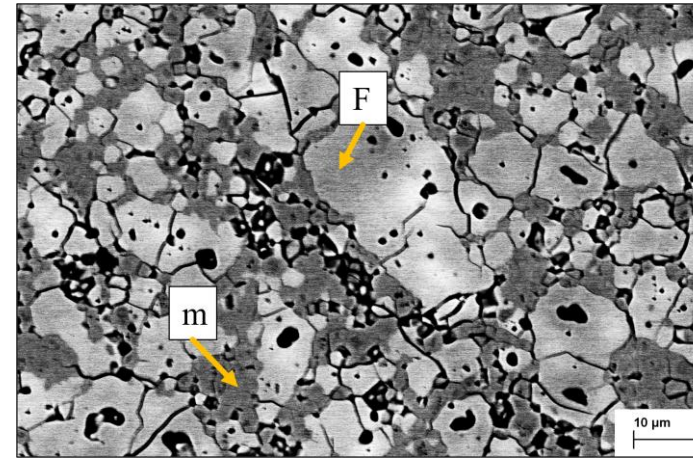
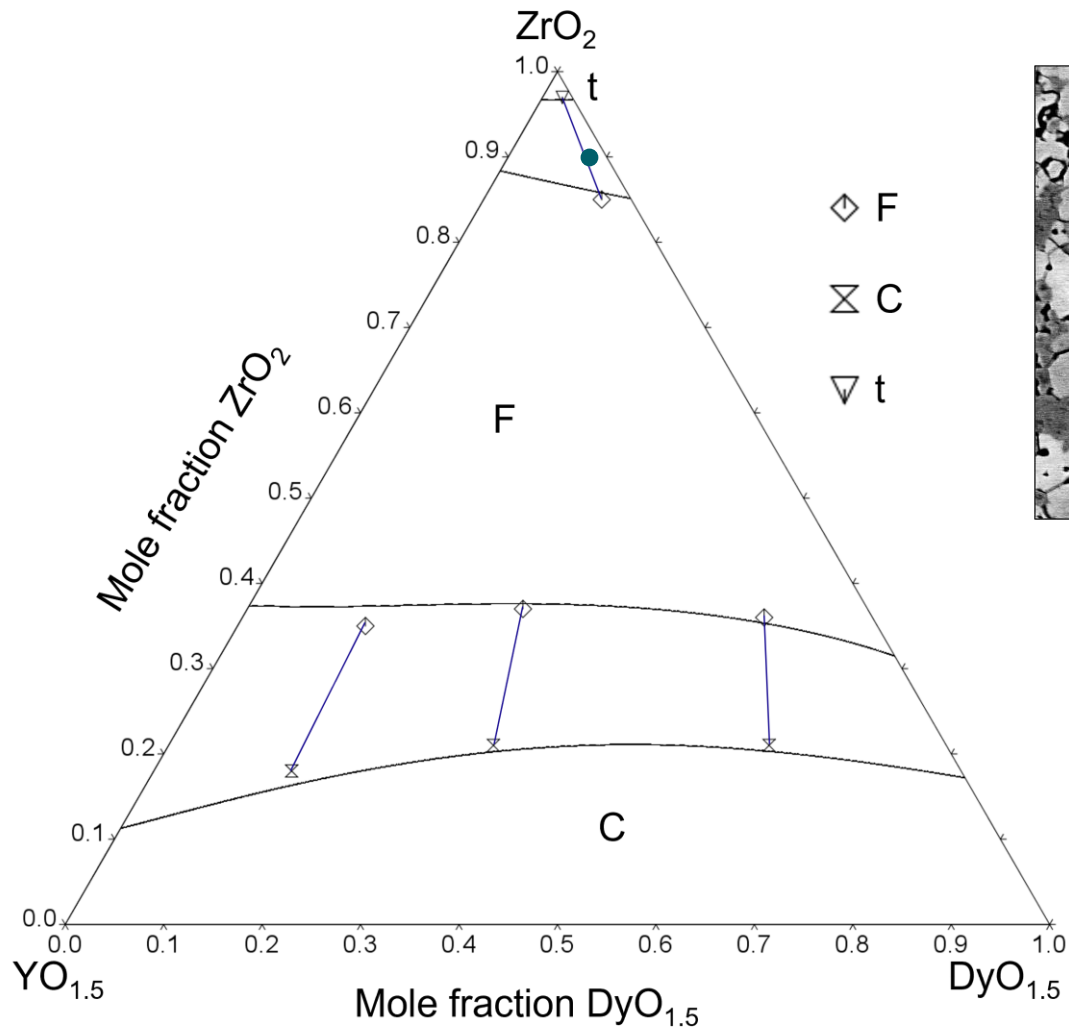
[20] A. Gavrish, *Inorg. Mat.* **1981**, 17, 1541.

[21] O. Korniienko et al., *Kharkiv Univ. Bull., Chem. Ser.* **2016**, 39-48.

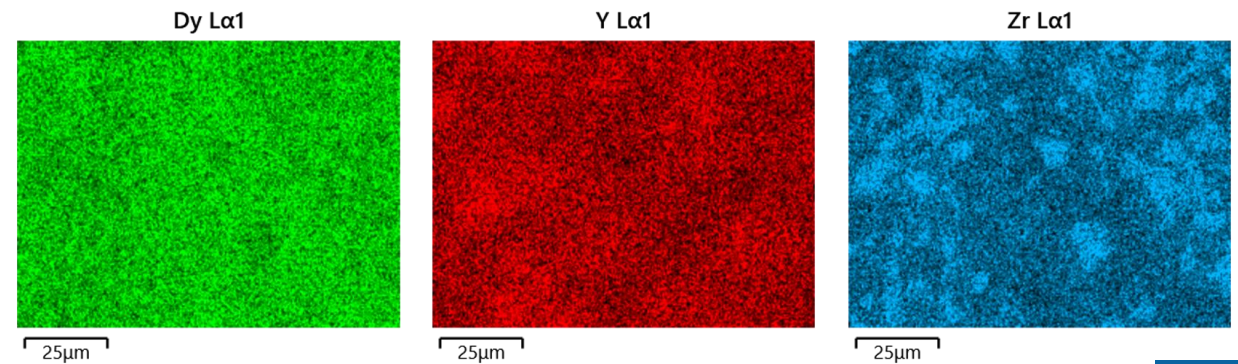
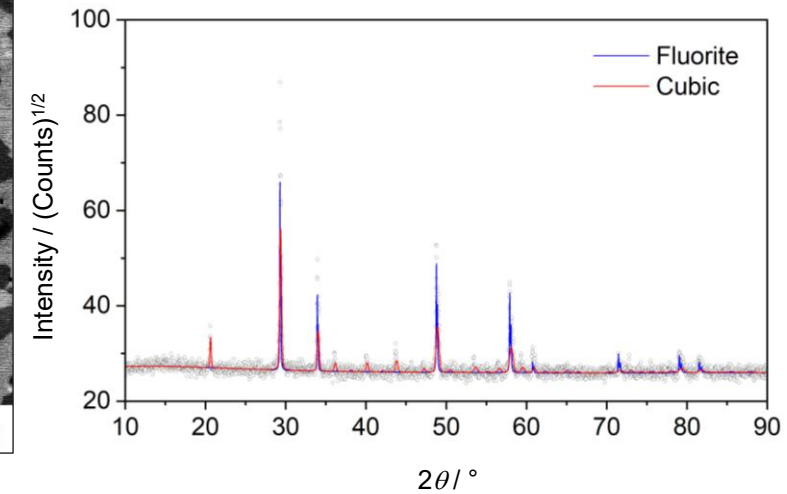
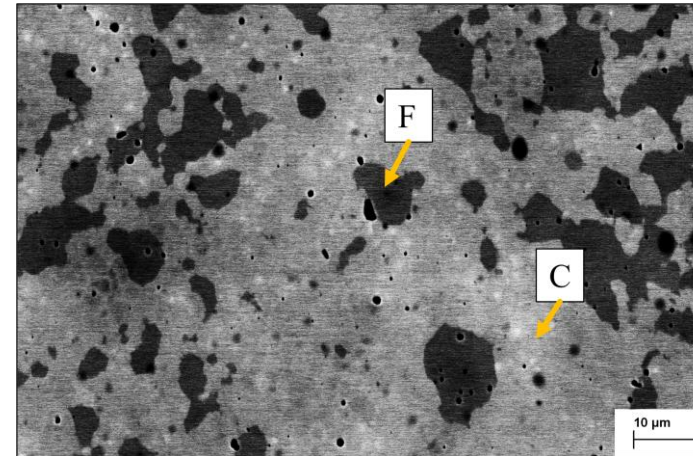
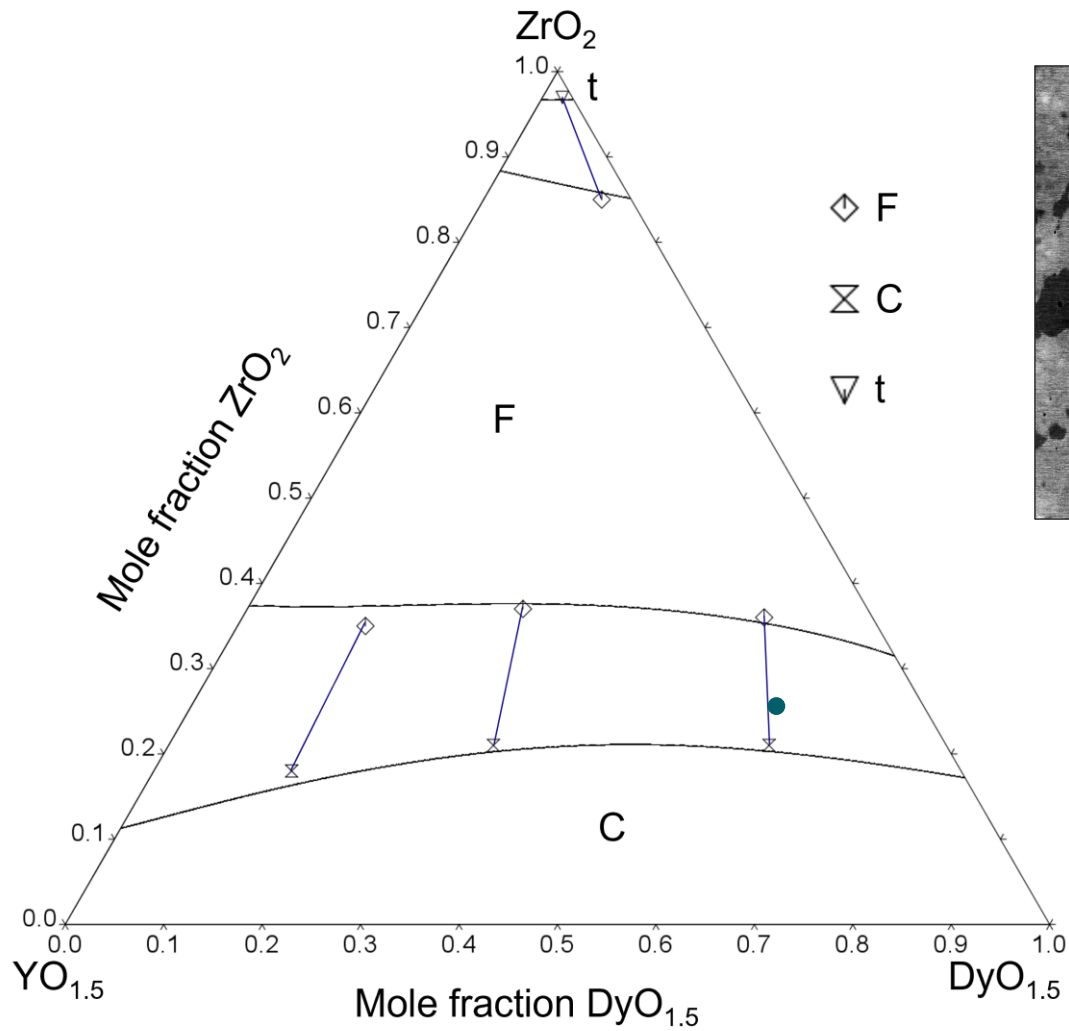
The $\text{ZrO}_2\text{-Dy}_2\text{O}_3$ system



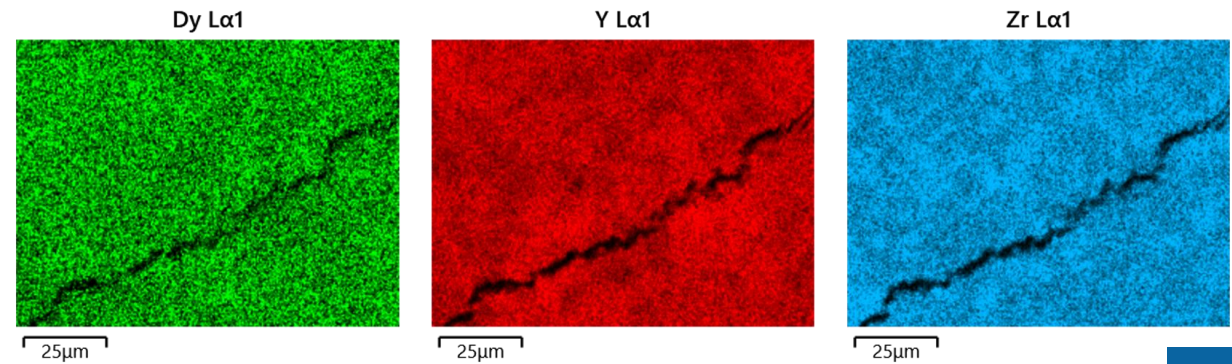
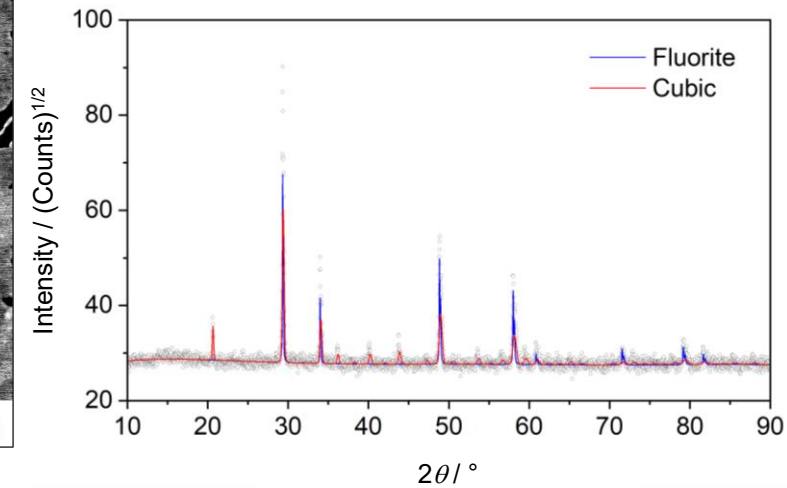
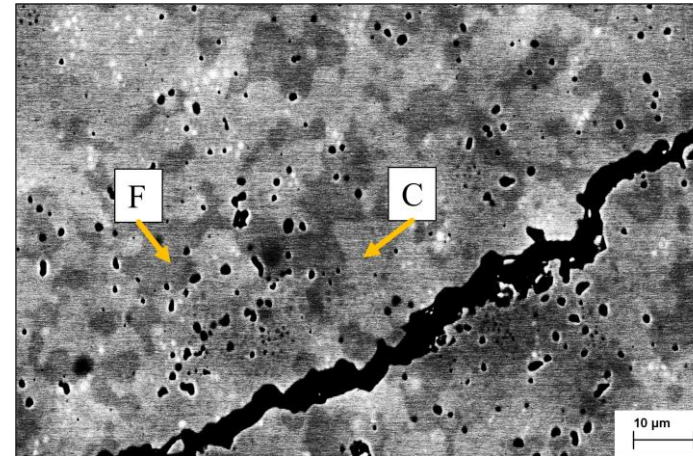
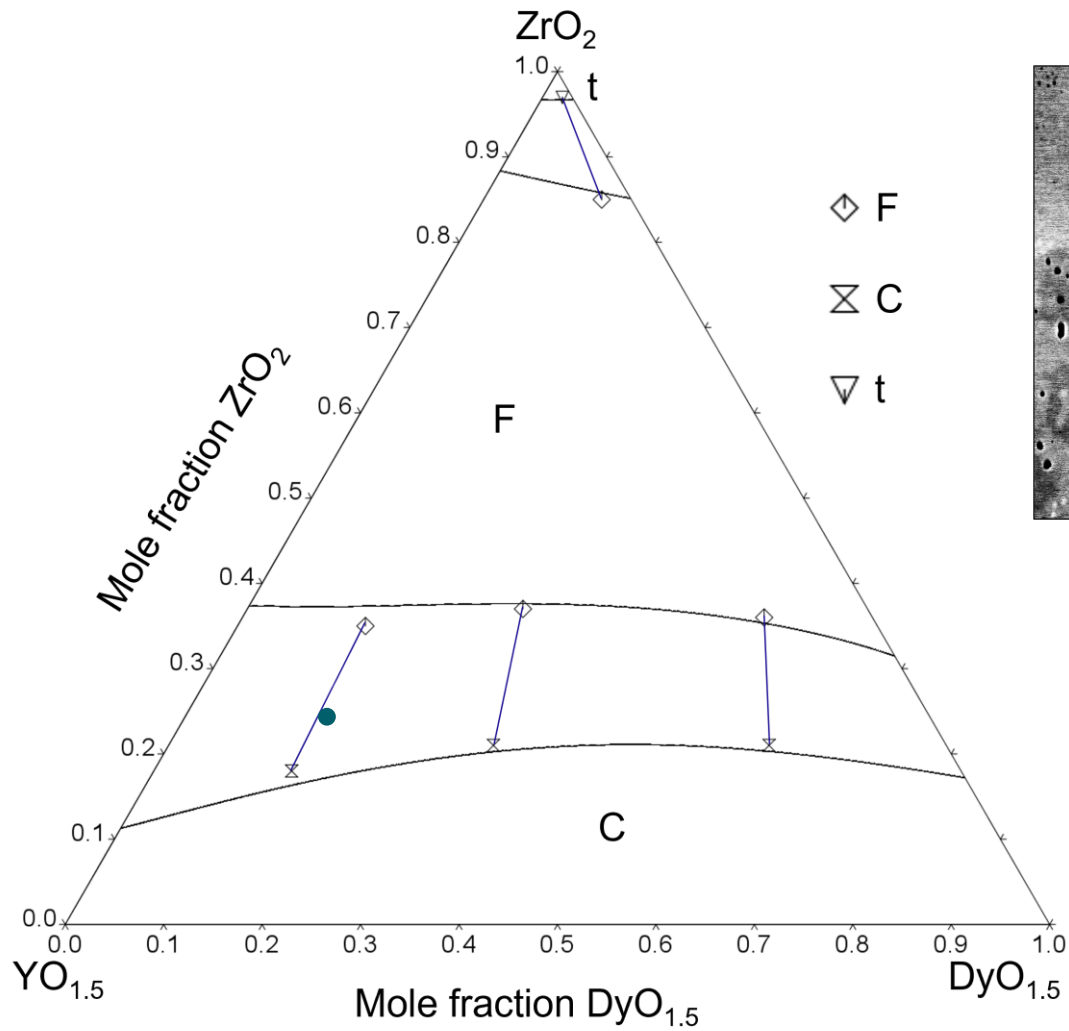
Isothermal section at 1773 K



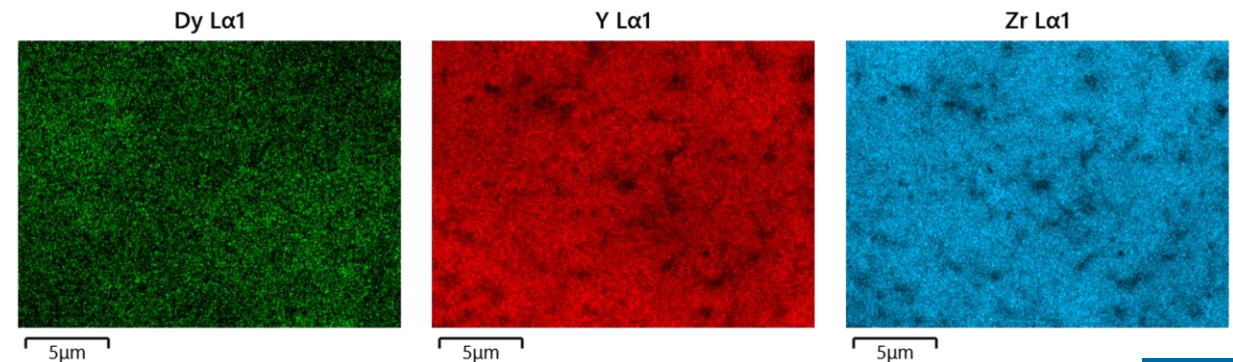
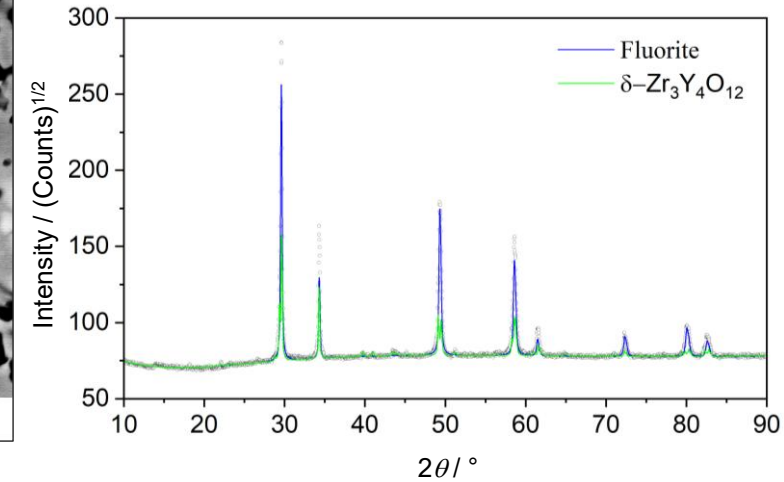
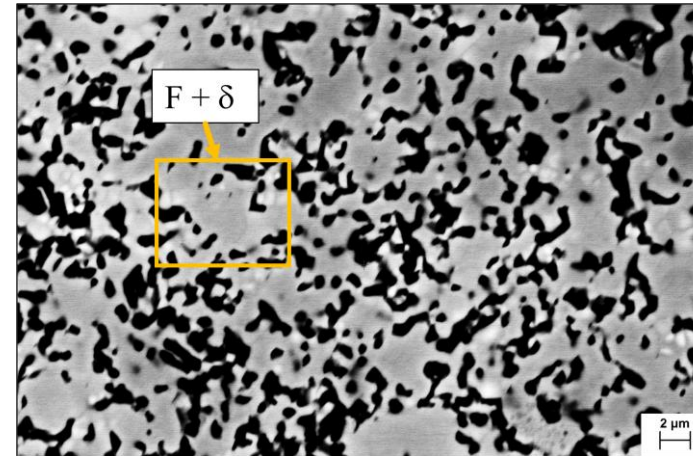
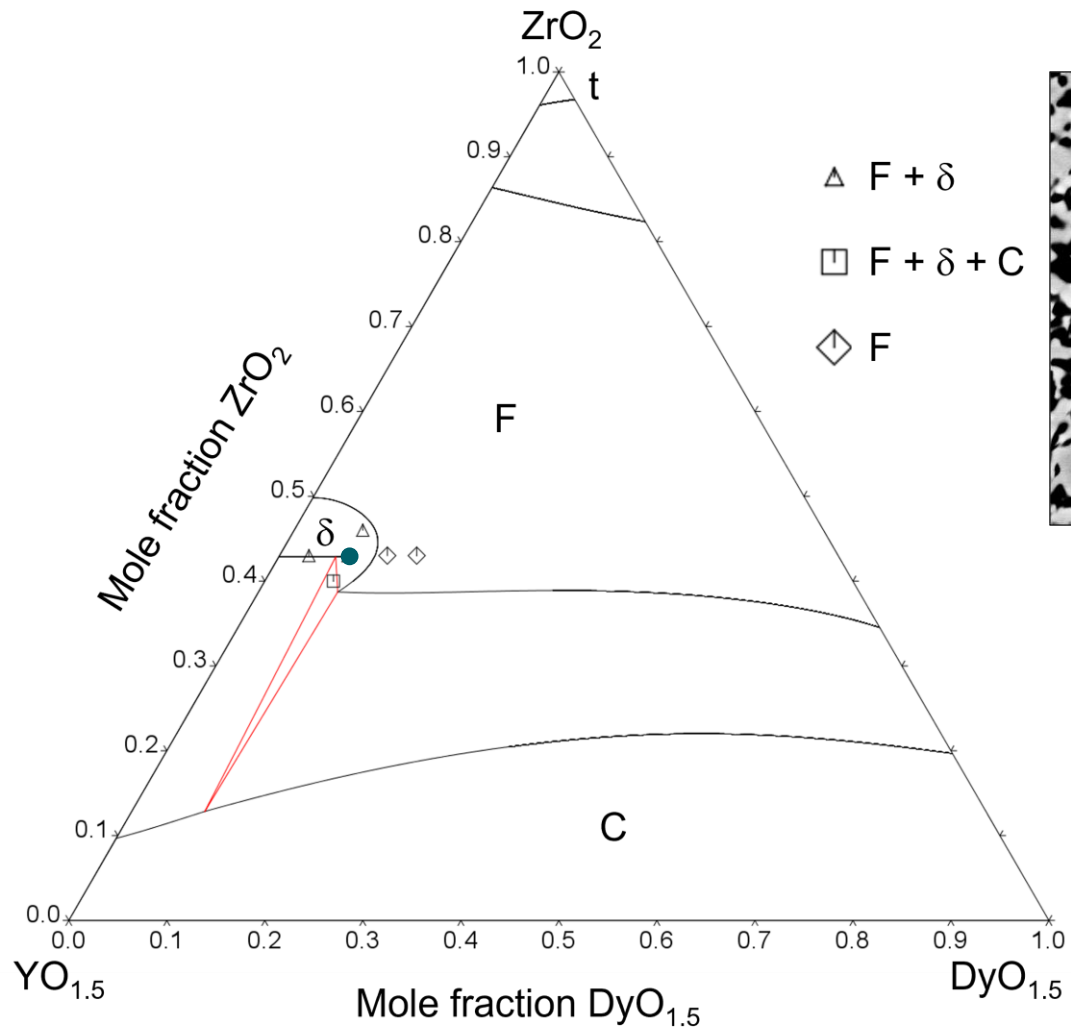
Isothermal section at 1773 K



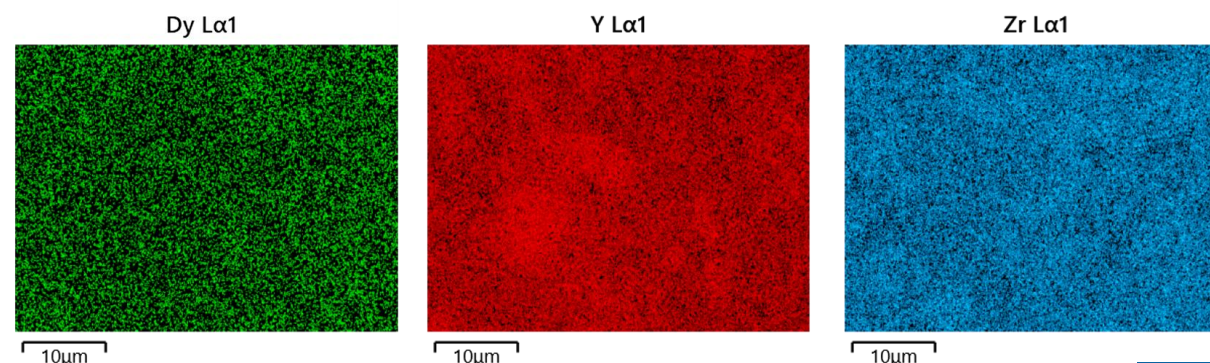
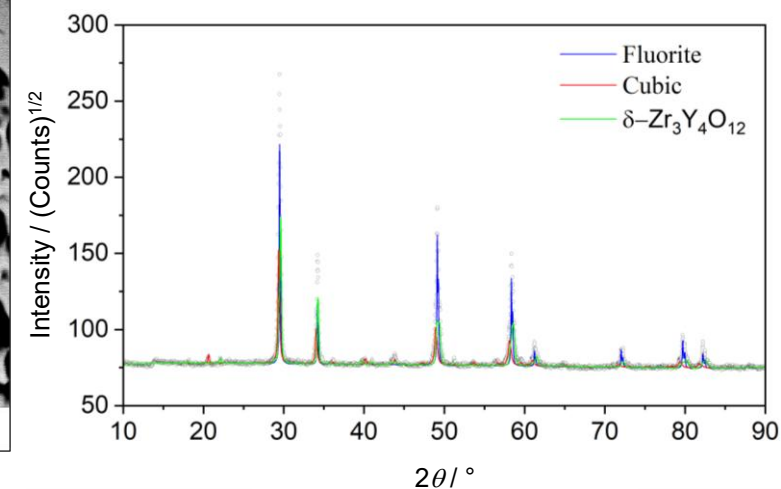
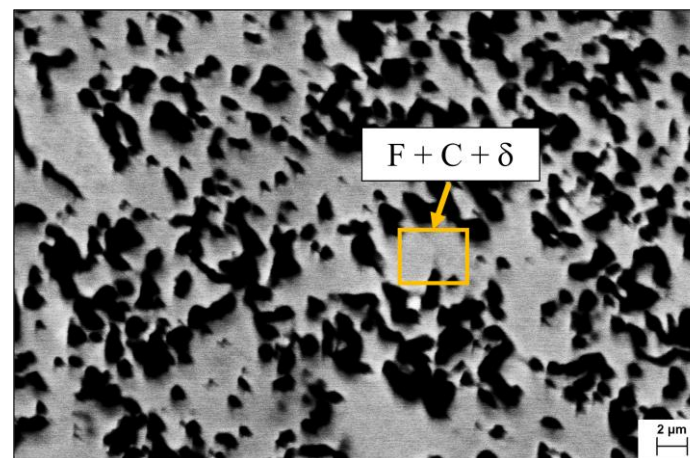
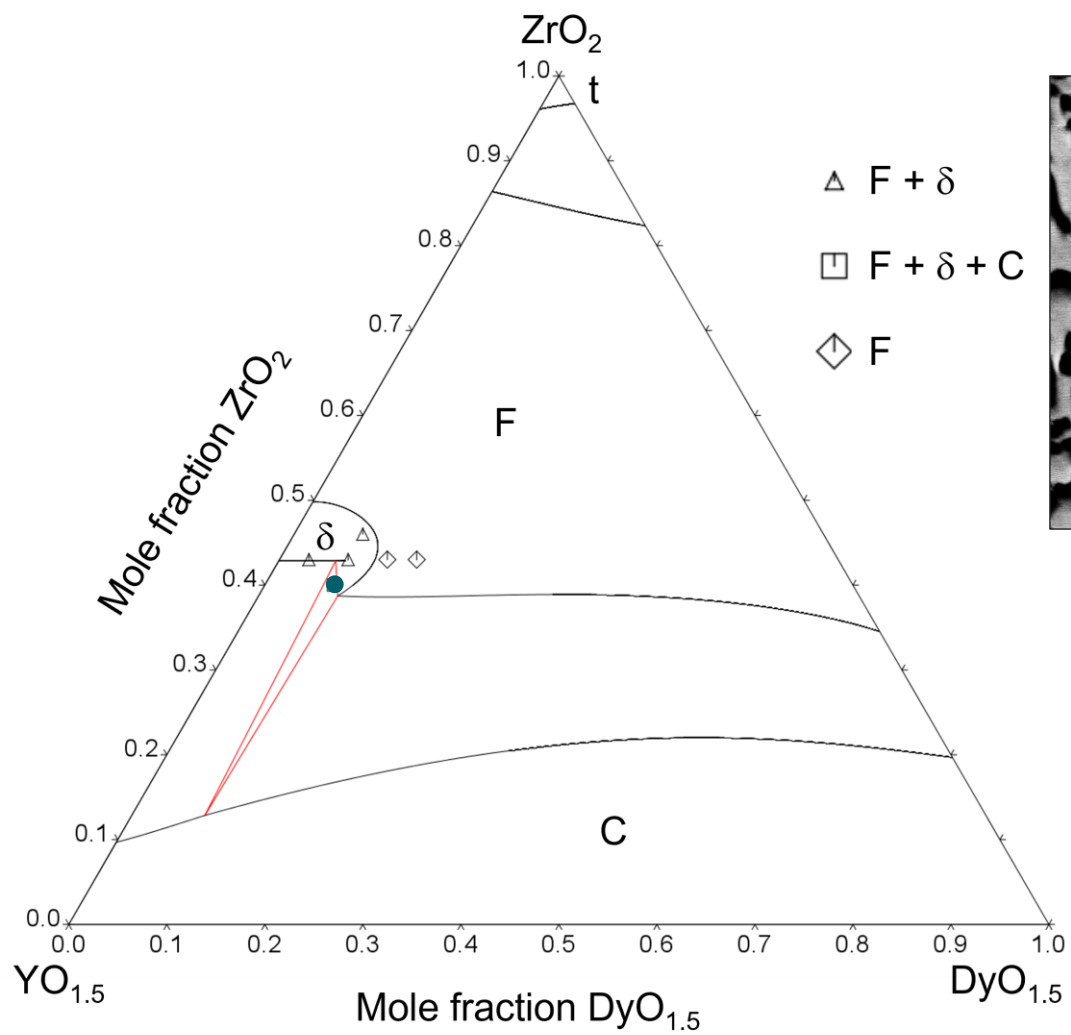
Isothermal section at 1773 K



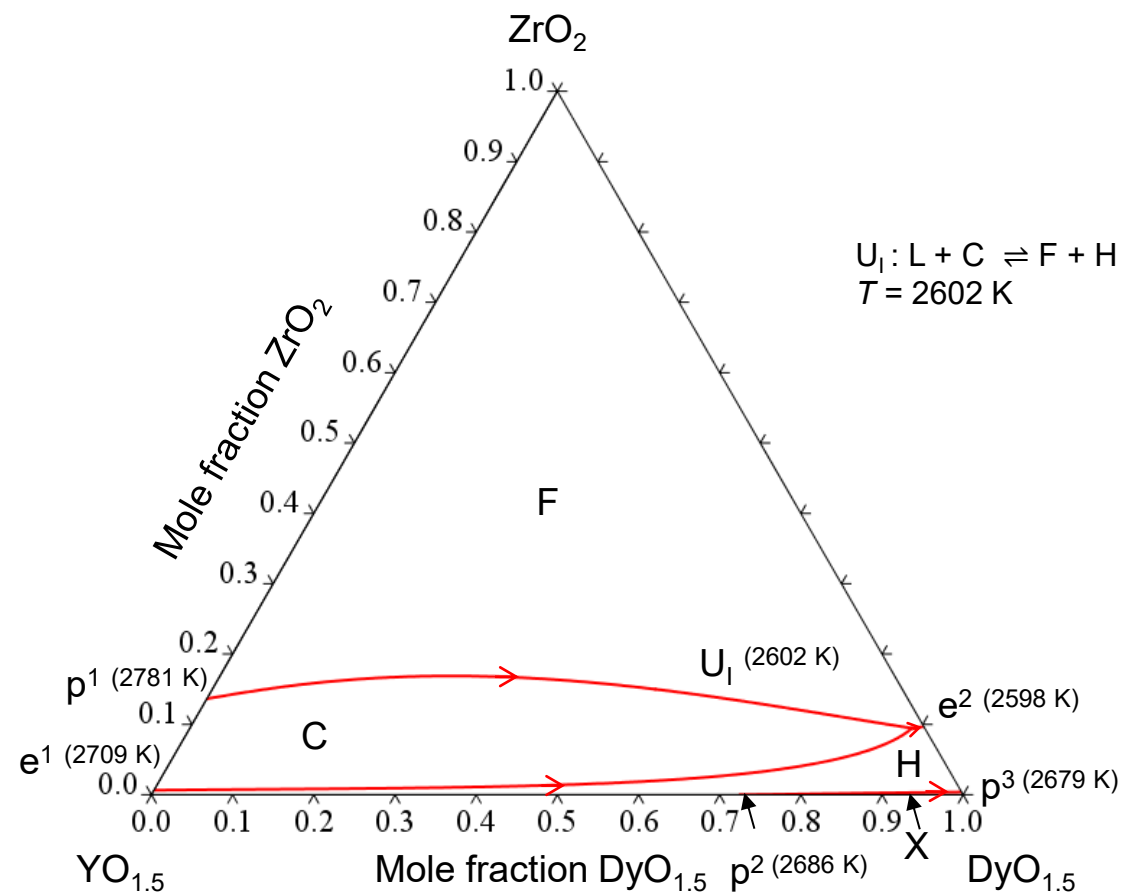
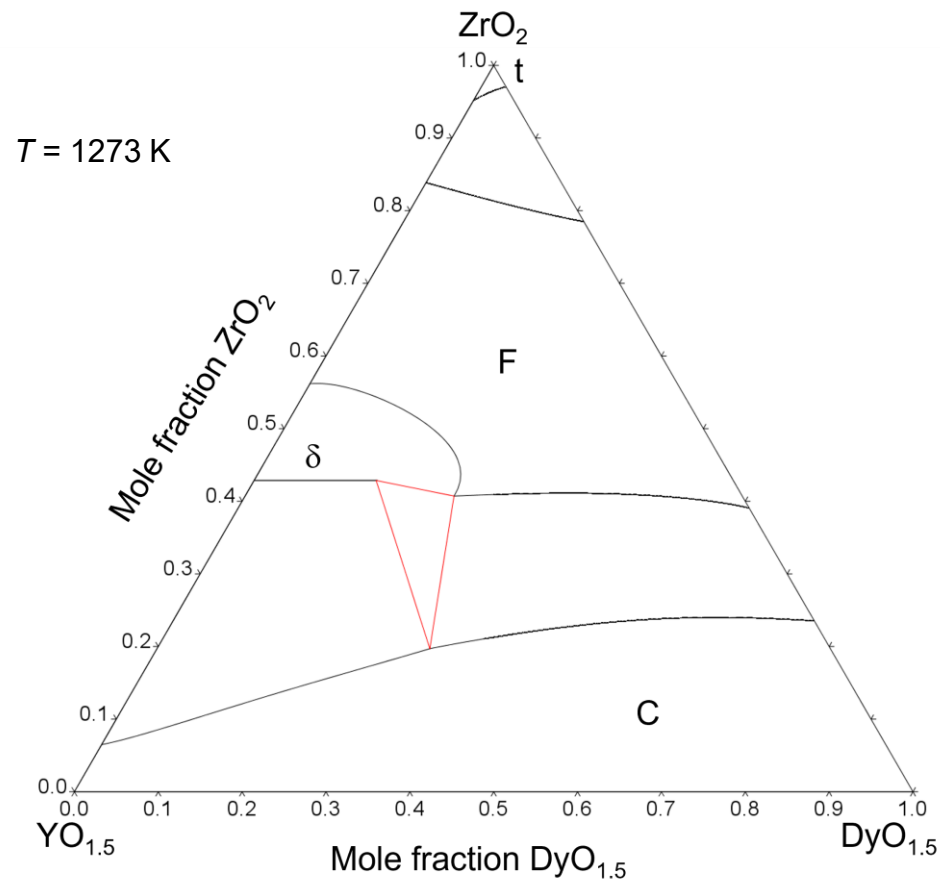
Isothermal section at 1573 K

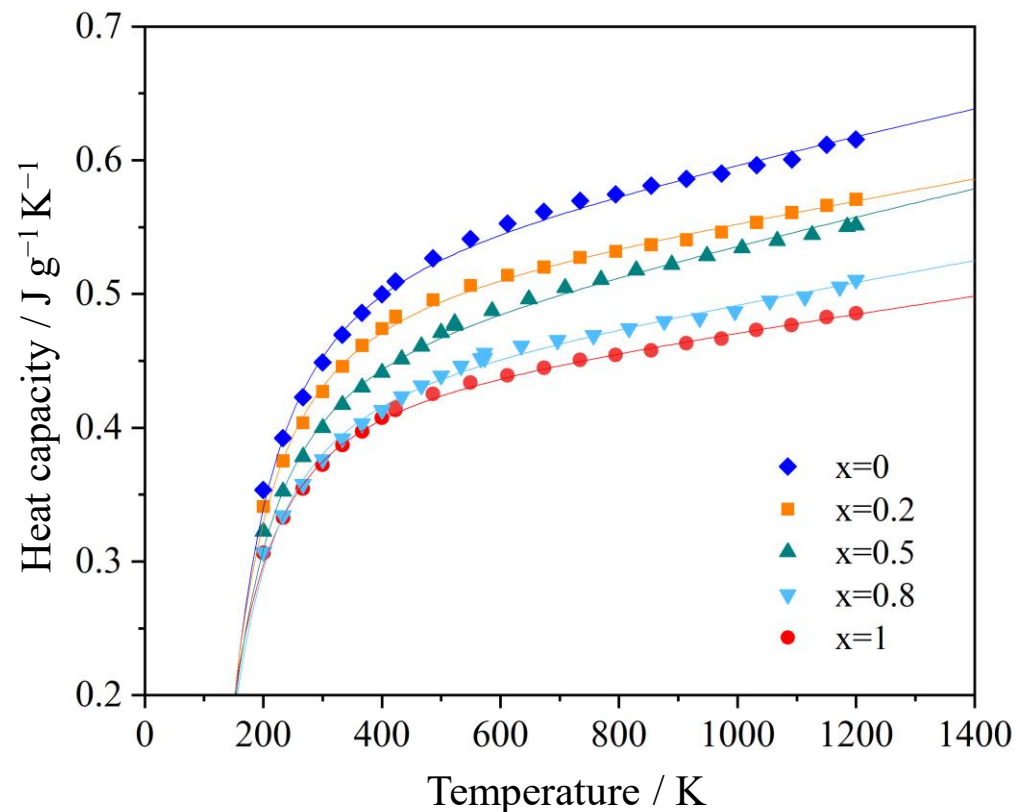
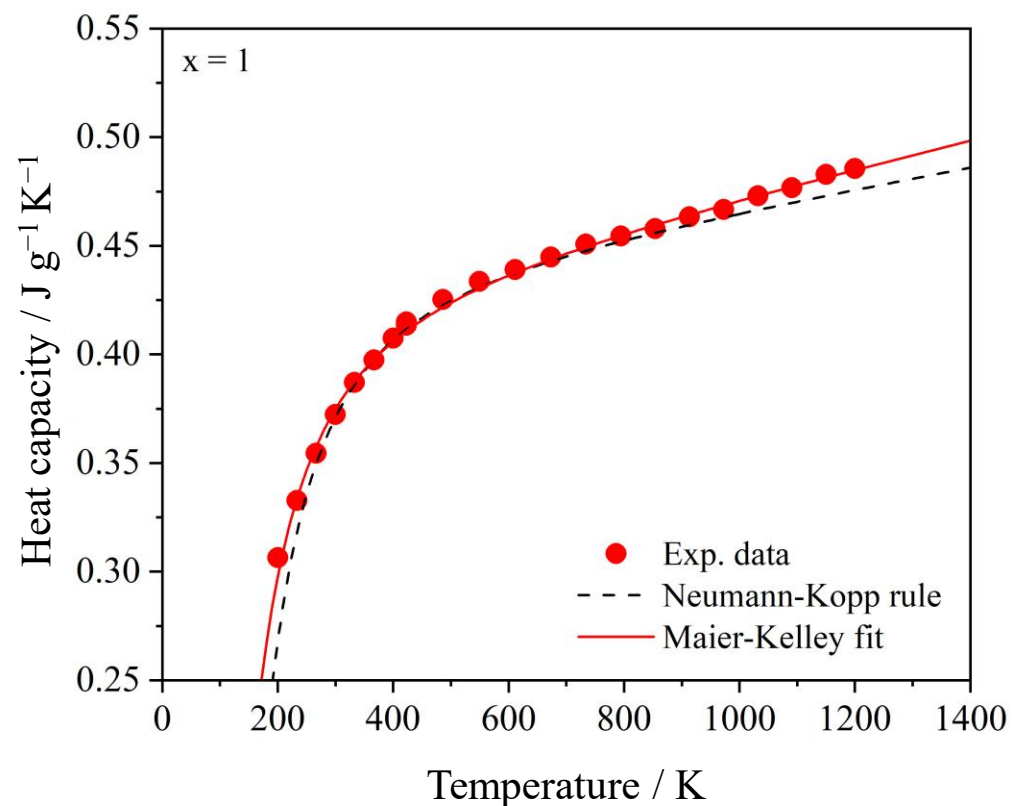


Isothermal section at 1573 K

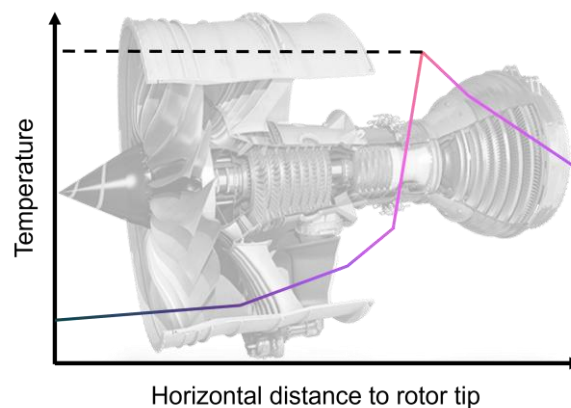
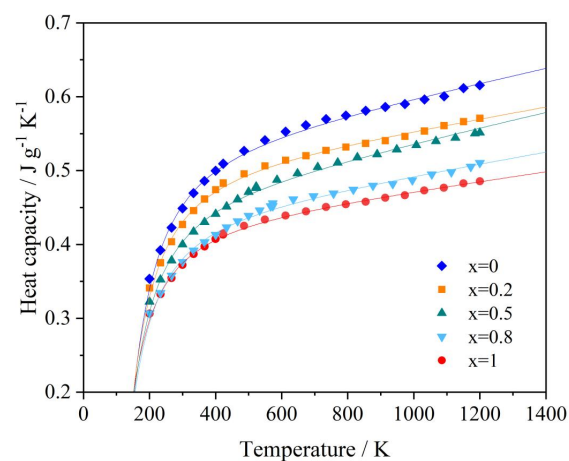
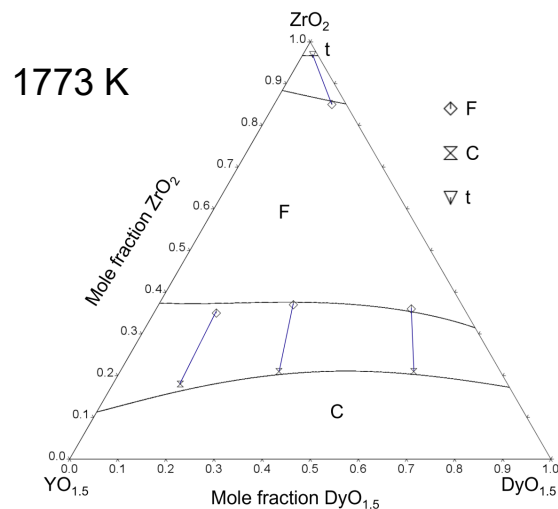
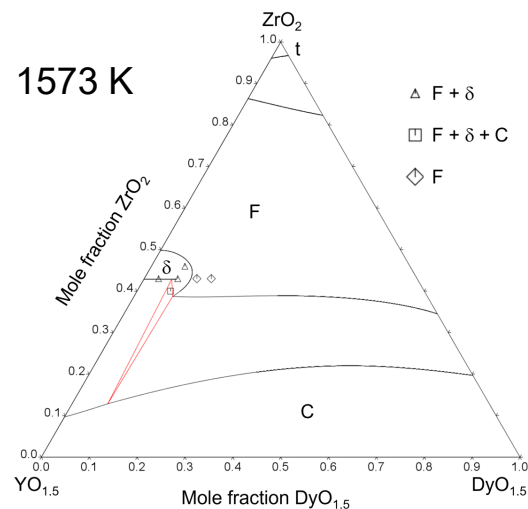


Low and high-temperature equilibria





$\text{Zr}_2(\text{Dy}_x\text{Y}_{1-x})_2\text{O}_7$ composition



Next systems to be investigated

$\text{ZrO}_2\text{-Dy}_2\text{O}_3\text{-Gd}_2\text{O}_3$
 $\text{ZrO}_2\text{-Dy}_2\text{O}_3\text{-Nd}_2\text{O}_3$
 $\text{ZrO}_2\text{-Dy}_2\text{O}_3\text{-Sm}_2\text{O}_3$

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Experimental and thermodynamic assessment of phase equilibria in the $\text{ZrO}_2\text{-YO}_{1.5}\text{-DyO}_{1.5}$ system[☆]

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Acknowledgements



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