High-Performance Materials for Next Generation Thermal Barrier Coatings in the System ZrO_2-HfO_2-Y_2O_3-Ta_2O_5

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Motivation

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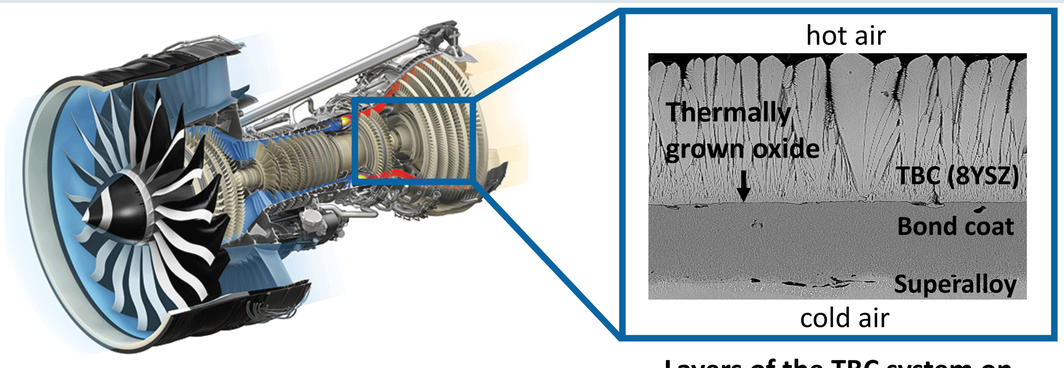
- ZrO_2-HfO_2-Y_2O_3-Ta_2O_5 is a promising material system regarding thermal barrier coating (TBC) applications
  - Extended tetragonal phase stable ZrO_2-rich phase field
  - Extended $YTaO_4$ phase field shows phase stability up to 1450 °C and low thermal conductivity
- Lack of thermochemical, thermodynamic and phase diagram data



TBC application in airplane turbines. [1]

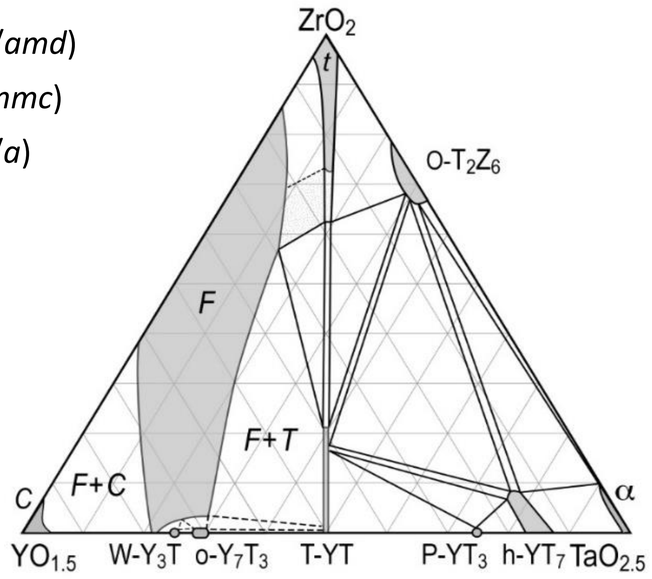
Layers of the TBC system on Ni-based superalloy.

Phase diagram ZrO_2-$YO_{1.5}$-$TaO_{2.5}$ system

2

The quasi-ternary system was determined experimentally, [2] thermodynamic data and the sub-systems are being investigated [3-5]

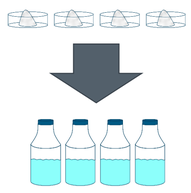
α = $TaO_{2.5}$ tetragonal ($I4_1/amd$)
t = ZrO_2 tetragonal ($P4_2/nmc$)
T = $YTaO_4$ tetragonal ($I4_1/a$)
F = ZrO_2 cubic ($Fm\bar{3}m$)
C = $YO_{1.5}$ cubic ($Ia\bar{3}$)
O-T_2Z_6 = $Ta_2Zr_6O_{17}$
o-Y_7T_3 = $Y_7Ta_3O_{18}$
h-YT_7 = YTa_7O_{19}
P-YT_3 = YTa_3O_9
W-Y_3T = Y_3TaO_7
T-YT = $YTaO_4$



Isothermal section of the ZrO_2-$YO_{1.5}$-$TaO_{2.5}$ system at 1500 °C. [2]

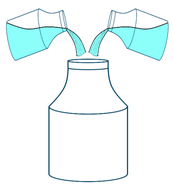
Synthesis: Co-precipitation route

3



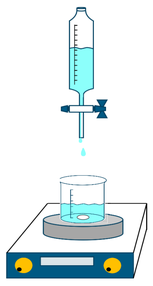
Step 1

Preparation of precursor solution



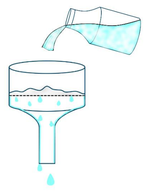
Step 2

Stoichiometric mixture of solutions



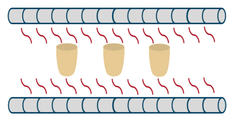
Step 3

Precipitation of hydroxides in ammonia solution



Step 4

Filtering products



Step 5

Drying, calcination and heat treatment

Courtesy to P. Hutterer

Outlook

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- XRD, SEM and EDS measurements for identification of phase and chemical compositions
- Specific heat capacity measurements for thermodynamic modelling and calculation of thermal conductivity
- DTA measurements for phase transition and melting temperatures
- In collaboration with TU Bergakademie Freiberg calculations of the quaternary phase diagram via CALPHAD method

HfO_2-$YO_{1.5}$-$TaO_{2.5}$ system

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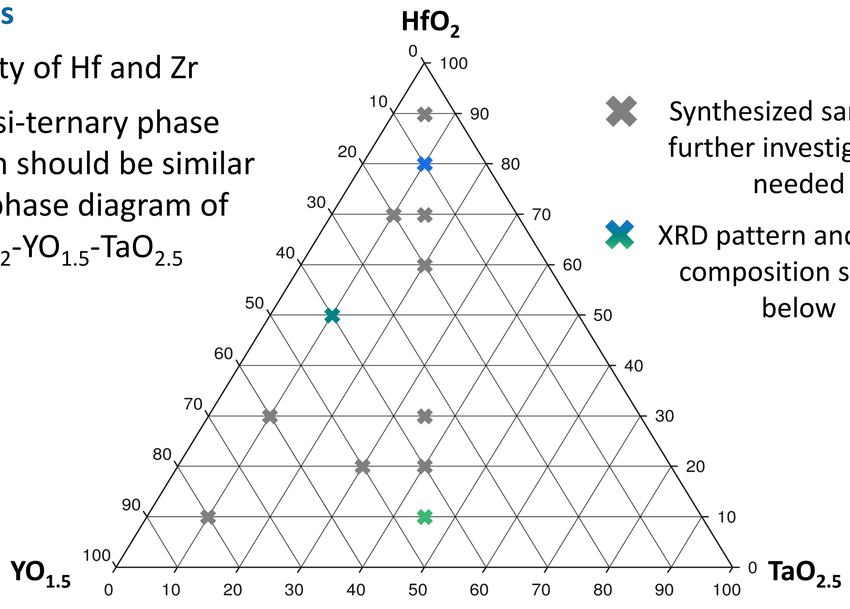
Hypothesis

- Similarity of Hf and Zr

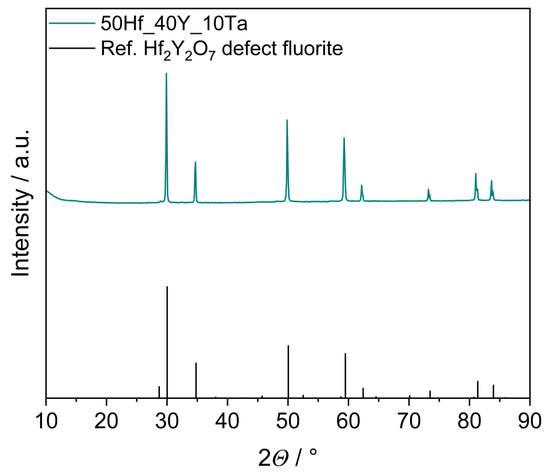
  → Quasi-ternary phase diagram should be similar to the phase diagram of the ZrO_2-$YO_{1.5}$-$TaO_{2.5}$ system



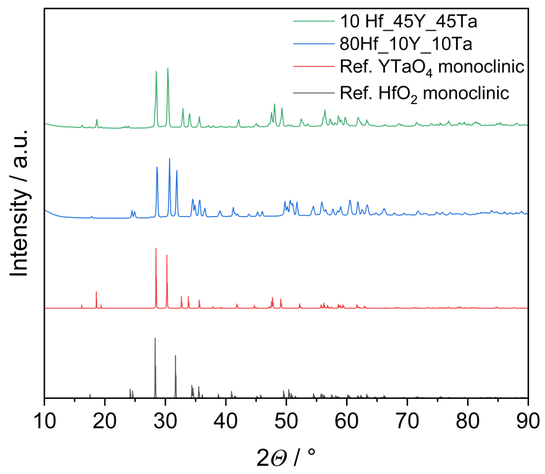
Tentative phase diagram of the HfO_2-$YO_{1.5}$-$TaO_{2.5}$ system at 1500 °C.

XRD measurements

- Tetragonal phase of HfO_2 appears at temperatures > 1700 °C, deviation from hypothesis expected



XRD pattern of a single-phase sample heat treated at 1500 °C for 100 h in air.



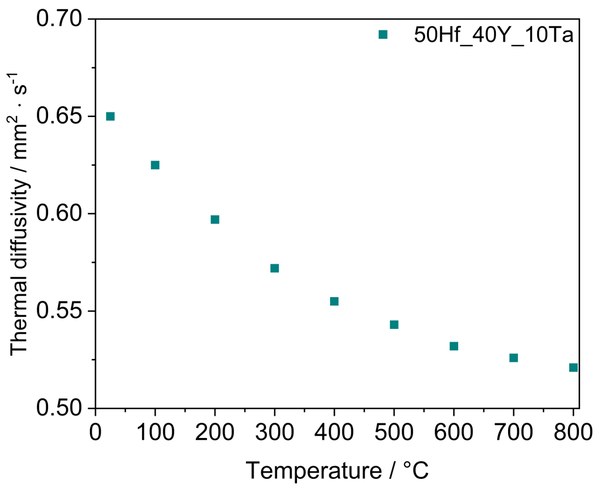
XRD pattern of compositions along the quasi-binary HfO_2-$YTaO_4$ heat treated at 1500 °C for 100 h in air.

Laser-Flash measurements

- Method to measure thermal diffusivity

  → For determination of thermal conductivity knowledge of density and specific heat capacity is necessary
- State of the art material (8YSZ) has a thermal diffusivity of 0.60-0.80 $mm^2 \cdot s^{-1}$ [6]

  → 0.52-0.65 $mm^2 \cdot s^{-1}$ obtained in measurement



Laser-Flash measurements of a single-phase sample heat treated at 1500 °C for 100 h.

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[2] C. Macauley *et al.*, *J Eur. Ceram. Soc.* **2017**, *37*, 4888-4901.
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