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Thermal Expansion of Yttria Stabilized Zirconia

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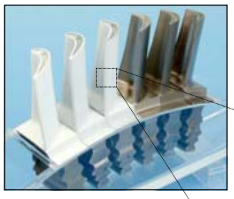
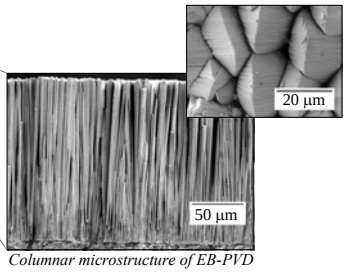
Introduction

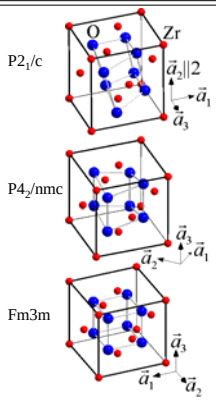
Today the state of the art material for Thermal Barrier Coatings (TBCs) is Yttria Stabilized Zirconia (YSZ). As shown in the phase diagram by Scott [1], different polymorphs of YSZ can be obtained by varying the Yttria content. Thereby monoclinic Yttria Stabilized Zirconia crystallises in space group $P2_1/c$, tetragonal Partially Yttria Stabilized Zirconia (PYSZ) in space group $P4_2/nmc$ and cubic Full Yttria Stabilized Zirconia (FYSZ) in space group Fm3m. In most cases, far from any phase transitions, the linear approximation for thermal expansion turned out to be an adequate approach. In the monoclinic phase (crystal class 2/m) zirconia exhibits four independent tensor coefficients, whereas in the tetragonal (4/mmm) and the cubic phase (m3m) there are only two and one coefficients, respectively. It is remarkable, that in the literature only little is known about the tensor coefficients of thermal expansion in YSZ. Moreover, existing data sets of thermal expansion of the different zirconia polymorphs are partial inconsistent. Thermal expansion data were obtained from Neutron and X-ray powder diffraction experiments.

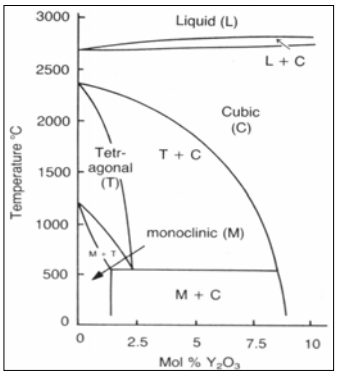


150 kW EP-PVD coater

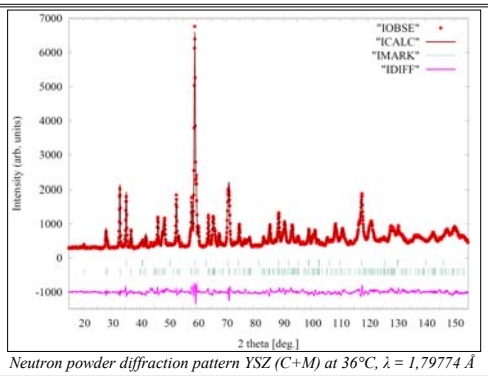


Columnar microstructure of EB-PVD PYSZ coating from a turbine blade [2]

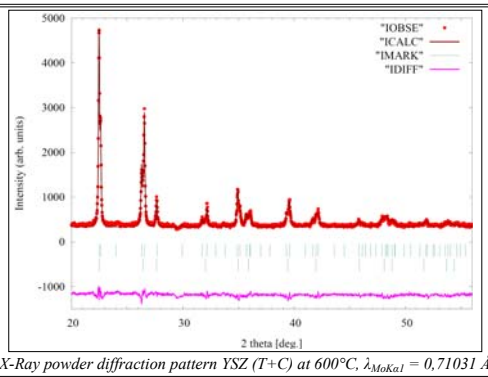




Phase diagram by Scott [1]



Neutron powder diffraction pattern YSZ (C+M) at 36°C, λ = 1,79774 Å



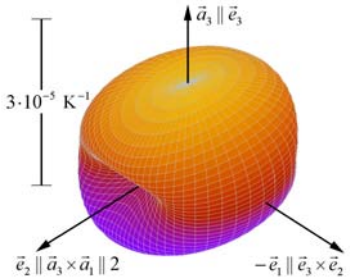
X-Ray powder diffraction pattern YSZ (T+C) at 600°C, λ_{MoKa1} = 0,71031 Å

Linear thermal Expansion: $L_i'(T) = L_i'(T_0)[1+\alpha_{ii}'(T-T_0)]$

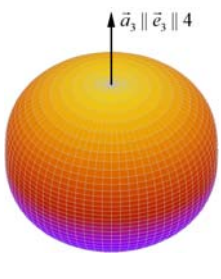
Neumann principle:

$$\underline{\underline{\alpha}}_{ij}^{M} = \begin{pmatrix} \alpha_{11} & 0 & \alpha_{13} \\ 0 & \alpha_{22} & 0 \\ \alpha_{13} & 0 & \alpha_{33} \end{pmatrix} \qquad \underline{\underline{\alpha}}_{ij}^{T} = \begin{pmatrix} \alpha_{11} & 0 & 0 \\ 0 & \alpha_{11} & 0 \\ 0 & 0 & \alpha_{33} \end{pmatrix} \qquad \underline{\underline{\alpha}}_{ij}^{C} = \begin{pmatrix} \alpha_{11} & 0 & 0 \\ 0 & \alpha_{11} & 0 \\ 0 & 0 & \alpha_{11} \end{pmatrix}$$

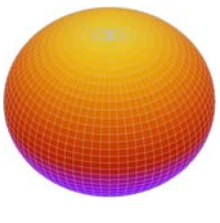
Representation surface:



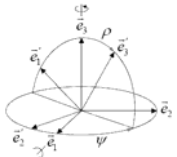
$$\alpha_{33}^{*M}(\rho,\psi) = \cos^2\psi \sin^2\rho\alpha_{11} + \sin^2\psi \sin^2\rho\alpha_{22} + \cos^2\rho\alpha_{33} + \sin(2\rho)\cos\psi\alpha_{23}$$



$$\alpha_{33}^{*T}(\rho,\bullet) = \sin^2\rho\alpha_{11} + \cos^2\rho\alpha_{33}$$



$$\alpha_{33}^{*C}(\bullet,\bullet) = \alpha_{11}$$



$\vec{e}_3 \parallel \vec{a}_3 \quad \vec{e}_2 \parallel \vec{a}_3 \times \vec{a}_1 \quad \vec{e}_1 \parallel \vec{e}_2 \times \vec{e}_3$

Conclusion

- High temperature X-ray diffraction and Neutron diffraction is a good method for evaluating thermal expansion coefficients of YSZ
- The thermal expansion coefficients of the cubic and tetragonal phase are very similar to each other
- The thermal expansion coefficients of the cubic and tetragonal phase differ significantly from the monoclinic phase
- Moreover the thermal expansion coefficients depend on the resulting phase and are nearly independent of the Yttria content
- Phase transformations to the monoclinic phase have to be avoided because its completely different thermal expansion behaviour necessarily leads to failure of the components

[1] H. G. Scott, J. Mater. Sci. **10,** 1527 (1975).

[2] A.F. Renteria, Doctoral thesis, Fakultät für Georessourcen und Materialtechnik RWTH Aachen, 2006.