<u>Performance Comparisons between Thermal Barrier Coating (TBC)</u> <u>Compositions at various Temperatures and Proportions</u>

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Introduction

TBC's are designed to insulate structural elements below it from the additional thermal stressed being placed upon modern gas turbine engines. Ensuring they are operating within their design parameters is essential in lengthening service lifespan of hot section components ^{1, 2}.

Figure 1 | Phase names and compositions present in YSZ, CMAS Systems¹

Туре	Name	Nominal formula
Intrinsic crystallization	Anorthite	$CaAl_2Si_2O_8$
	Diopside	CaMgSi ₂ O ₆
	Cristobalite, tridymite	SiO ₂
	(Pseudo)wollastonite	CaSiO ₃
	Melilite	(Ca) ₂ (Al,Mg)(Al,Si)SiO ₇
	Spinel	$MgAl_2O_7$
Reprecipitation	Fluorite	$(Zr,RE,Ca)O_{1.x}$
	Tetragonal ZrO ₂	$(Zr,RE,Ca)O_{1.x}$
	Celsian	$(Ba,Sr,Ca)Al_2Si_2O_8$
Reactive crystallization	Zircon	ZrSiO ₄
	CaZr-cyclosilicate	$Ca_2ZrSi_4O_{12}$
	Calcium zirconate	CaZrO ₃
	Apatite	$(Ca,RE)_4(RE,Zr)_6(SiO_4)_6O_2$
	Garnet	(Ca,RE,Zr) ₃ (Zr,Ti,Mg,Al,Fe) ₂ (Si,Al,Fe) ₃ O ₁₂
	Cuspidine	(RE,Ca,Hf,Mg) ₄ (Si,Al) ₂ O _{9.x}
	CaRE-cyclosilicate	$Ca_3RE_2Si_6O_{18}$
	Silicocarnotite	$Ca_3RE_2Si_3O_{12}$

Figure 2| Schematic of TBC and TBC Coatings¹







- Equilibrium data for the systems shown here were generated using the Calculation of Phase Diagrams (CALPHAD) methodology through ThermoCalc.
- Database used was TCOX 7, a metal oxide solution simulator. CALPHAD utilizes multiple different chemical and physical properties such as crystallography and available free energy.
- Figure 5 shows melt composition if 100% pure. Changes to phases developed was observed upon addition of TBC. Desired phases include reactive crystallization products which have a geometry favourable to impede melt progress.
- Figure 6 demonstrates ThermoCalc's oxygen activity limits with a more complex system. A CAS system was selected with 10⁻¹⁴ oxygen activity to ensure solution convergence.



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multi-valency affected the model more than anticipated ⁵.

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