



Database name: SGTE Thermal Barrier Coating database
Database acronym: STBC1 **Database version:** 1.1
Database owner: Scientific Group Thermodata Europe
Database segment: Thermal Barrier Coatings

Brief description

STBC1 can be applied in many different fields of technology (for instance, yttria-stabilised-zirconia (YSZ), solid electrolyte (fluorite), thermal barrier coating (TBC using tetragonal oxides), and so forth), and most importantly the use of this database can further enhance such technologies.

Applications

Research, design and engineering of thermal barrier coatings.

Included Elements

Al Gd O Y Zr

Included Phases

CORUNDUM	M2O3A	M2O3H	MAM	OPYRO
FLUORITE	M2O3B	M2O3X	MAP	TETR
IONIC_LIQ	M2O3C	MAG	MONO	RHOMB_B

Assessed Systems

The current version STBC1 covers many complex solution phases, *e.g.*, fluorite_ZrO₂, tetragonal_ZrO₂, monoclinic_ZrO₂, cubic_M₂O₃C, cubic_M₂O₃X, monoclinic_M₂O₃B, hexagonal_M₂O₃A, hexagonal_M₂O₃H, δ_Zr₃Y₄O₁₂, pyrochlore_Gd₂Zr₂O₇, monoclinic_LnAM, perovskite_LnAP, garnet_LnAG, corundum, and liquid. It utilizes the Two-Sublattice Ionic Liquid Model for the liquid mixture phase, and the Compound-Energy Formalism (CEF) with ionic constraints for various solid solution phases.

Validation

This database has been developed by MPI-MF, PML Stuttgart, Germany and been recently approved/released by SGTE as a so-called "SGTE application database". It contains critically-assessed thermodynamic data for the Al₂O₃-Gd₂O₃-Y₂O₃-ZrO₂ system, based on various experimental information such as phase equilibria (available from 1100 to 1300°C), as well as calorimetric measurements and vapour pressure determinations (over a wider temperature-composition range).

Beside phase equilibrium and phase diagram calculations, the Thermo-Calc (TCC/TCW) software also enables some specific calculations using this database, such as T₀-lines for diffusionless transformations (*e.g.*, fluorite ⇌ tetragonal_M₂O₃A, tetragonal_M₂O₃A ⇌ monoclinic_M₂O₃B), driving forces for partitioning of non-equilibrium phase to equilibrium assemblage, and so on.

Note that it is not appropriate to use this database to calculate phase equilibria in metallic or metal-oxygen system and in those involving a gas phase.

Limits

Critical calculations must always be verified by equilibrium experimental data; it is the user's responsibility to verify the calculations but Thermo-Calc Software is interested to know about any significant deviations in order to improve any future release.

Scientific Models & References

See the Thermo-Calc Software reference list available at:

http://www.thermocalc.com/DOWNLOAD_AREA/References.html