



Database name: SGTE Thermal Barrier Coating database
Database acronym: STBC2 **Database version:** 2.2
Database owner: Scientific Group Thermodata Europe
Database segment: Thermal Barrier Coatings

Brief description

STBC2 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

IONIC_LIQ	CORUNDUM	M2O3R	RMAG	PYRO
FLUORITE	M2O3A	M2O3H	RMAP	ZR3Y4O12
MONO	M2O3B	M2O3X	RMAM	FCC_A1
TETR	M2O3C			

Assessed Systems

The current version STBC2.2 covers many complex solution phases, *e.g.*, fluorite_ZrO₂, monoclinic_ZrO₂, tetragonal_ZrO₂, corundum_M₂O₃, hexagonal_M₂O₃A, monoclinic_M₂O₃B, cubic_M₂O₃C, hexagonal_M₂O₃H, cubic_M₂O₃X, garnet_LnAG, monoclinic_LnAM, perovskite_LnAP, δ _Zr₃Y₄O₁₂, pyrochlore_Gd₂Zr₂O₇, as well as oxide-liquid and FCC (for pure Al or O in FCC_A1 structure). It utilizes the Two-Sublattice Ionic Liquid Model for the liquid mixture phase, and the Compound-Energy Formalism (CEF) with ionic constrains 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 software Thermo-Calc also enables some specific calculations using this database, such as T₀-lines for diffusionless transformations (*e.g.*, fluorite \leftrightarrow tetragonal_M₂O₃A, tetragonal_M₂O₃A \leftrightarrow 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

As in the spirit of the CALPHAD method, predictions can be made for multicomponent systems by extrapolation into multicomponent space of data critically evaluated and assessed based on binary, ternary and in some cases higher order systems. However, critical calculations must always be verified by equilibrium experimental data; it is the user's responsibility to verify the calculations but Thermo-Calc Software AB 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/Library.htm>