C2: Thermodynamic modelling

Thermodynamic modelling of ZrO₂-MgO materials and steel-ZrO₂ interfaces

Objectives, Research Project

Vision
Application of CALPHAD approach for development of thermodynamic database for ceramic material Mg-stabilised ZrO₂ (Mg-PSZ) including titan, manganese, and iron oxides to model interaction between TRIP steel, titan, and Mg-PSZ

Results Achieved

- Thermodynamic database development for steel including 11 elements: Fe, Cr, Mn, Ni, Mo, Ti, W, V, Si, C, N
- Modeling of order/disorder and magnetic contributions

Vertical section of phase diagram for the Fe-16Cr-7Mn-xNi system (x=0-16 mass. %)

- Experimental study of interaction between Mg-PSZ: Mg₂SiO₄ formed at the interface
- Thermodynamic calculations applied to determine conditions of Mg-PSZ destabilisation

Equilibrium phase diagram for the ZrO₂-MgO system

Equilibrium phase diagram for the MgO-FeO-Fe₂O₃ ternary system at 1433 K

- Database development for the ZrO₂-MgO-MnO-FeO-Ti₂O₃-TiO₂ system
- Evaluating the effect of titanium to phase relations at the interface between steel and Mg-PSZ
- Experimental investigation of phase relations in the ZrO₂-MnO system and assessment of thermodynamic parameters based on data obtained
- Experimental investigations of ceramic material and steel using thermal analysis methods DTA and dilatometry

Network

- Phase equilibrium data: A1, A5, A6, S1, and B1
- Ceramic powder for dilatometry and DTA, steel powder for DTA: A1 and A5
- X-ray diffraction: fluorite structure + tetragonal (13 %) + monoclinic (17 %) phases. After DTA amount of monoclinic phase reduced up to 5%

Milestones

IV 2013 ➞ Thermodynamic database development for ceramic material ZrO₂-MgO-TiO₂-Ti₂O₃
I 2014 ➞ Experimental study of the ZrO₂-MnO system and assessment of thermodynamic parameters
III 2015 ➞ Thermodynamic assessment of the Ti-Fe-O, Ti-Mn-O, and MgO-MnO-FeO systems and incorporation of results into the TiO₂-Ti₂O₃-MgO-FeO-MnO database
I 2016 ➞ Thermodynamic database development for the ZrO₂-TiO₂-Ti₂O₃-MgO-FeO-MnO system