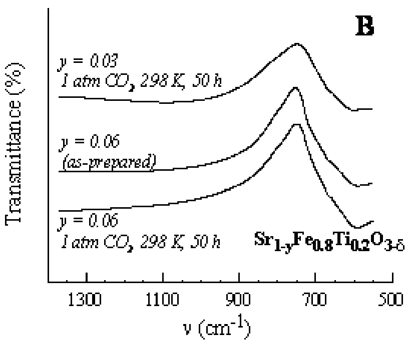
minor composition changes for major impact on tolerance to reactive gases

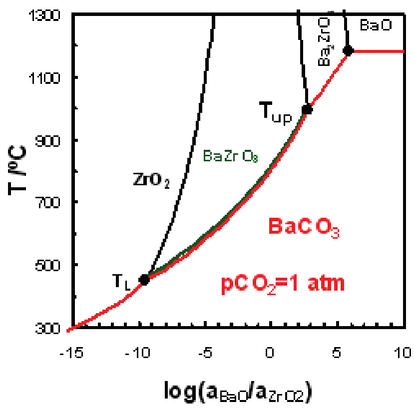
jorge frade[1], josé monteiro[1], ana brandão[1], isabel antunes[1], duncan fagg[2], glenn mather[3], josé grácio[2], vladislav kharton[1], andrei kovalevsky[1]

[1] ceramics and glass engineering department & CICECO, university of aveiro
[2] department of mechanical engineering & center for mechanical technology and automationTEMA, university of aveiro
[3] institute of ceramics and glass, CSIC, spain

Thermodynamic predictions are used to predict interaction of a variety of materials with reactive gases. It was demonstrated that minor composition changes suppress the activity of reactive components and play major impact on tolerance to reactive gases. This thermodynamic approach was also used as guideline for establishing stability ranges on thermal cycling, and to minimize the thermodynamic driving force for degradation in contact with gases.

Thermodynamic analysis of AO-BO_2-G systems (G=CO_2, H_2O, H_2S, etc.) provide guidelines for interpretation of resistance of $A^{II}B^{IV}O_3$-perovskites to reactive gases, with emphasis on materials with high technological relevance. The analysis demonstrated major differences between stability limits for materials with excess and deficiency of the reactive AO oxide, and corresponding upper and lower temperature limits for immunity to reactive gases. On combining these thermodynamic calculations for a variety of $A^{II}B^{IV}O_3$ perovskites, a high degree of





correlation between the stability limits and the Goldschmidt tolerance factor was demonstrated. These correlations allow reliable predictions to be obtained even for complex compositions and for cases when insufficient thermodynamic data prevent precise analysis.

The upper and lower temperature limits of stability ranges can be used to predict the evolution of reactions on cooling from high temperatures and also upon re-heating ABO_3 perovskites in reactive atmopsheres, as confirmed by IR, TG, etc.

Representative materials are used to confirm the applicability to components of solid state electrochemical systems proposed for conversion of hydrocarbon fuels, and is also being used for interactions of cements with CO_2 and/or humidity.