Thermodynamic Modeling of the SiO_2-B_2O_3-Na_2O system using CALPHAD method for SBN glasses

Post Doctoral position at CEA Saclay – Nuclear Energy Division

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Duration: 1 year Post-Doctoral position

Collaborations: This Post Doc is granted in the framework of the TOUGHGLASSES project funded by ANR in collaboration with:

- SPHYNX, SPEC, IRAMIS, CEA, Université Paris-Saclay
- IPR, Université de Rennes

Context and objectives:

Stress Corrosion Cracking (SCC) is one of the major issues in the glass industry. Making glasses tougher and less reactive to SCC is an important challenge in many areas (buildings, cars, dishes) along with being integral parts of heat resistant technologies, protection panels, low-carbon energies and satellites.

The aim of the ToughGlasses project concerns a fundamental study directed at understanding how to delay SCC in glasses via the structure.

Heat treating and leaching of SiO_2-B_2O_3-Na_2O (SBN) glasses can lead to porous glasses that can subsequently be used for functional glasses. However, their resistance towards stress corrosion cracking remains unknown. These porous glasses take advantage of the existence of several (2 or 3) miscibility gaps in the phase diagrams of the glasses. Scientists leach one or two phases to increase the porosity of the glass.

When looking at fracture and stress corrosion cracking, the miscibility gap may be associated with dramatic changes in the process zone around the crack tip, effectively diffusing stresses.

To the best of our knowledge, no one has examined the fracture properties or SCC of 2 or 3 phase demixed glasses outside the context of the preliminary/proof of concept works presented herein. Thus, it is of great interest to study SBN samples within this zone of the miscibility gap.

A more pointed statement of this Post Doc proposal is to study the effect of miscibility gap compositions on the toughness of such materials through thermodynamic considerations. These fundamental issues in the glass industry will be treated by two complementary approaches: an experimental study on miscibility gaps in SBN glasses and a thermodynamic modeling of the SBN system.

Laboratory:

LM2T laboratory is part of the Nuclear Energy Division (DEN). This division provides public authorities and industries with innovative ideas and the expertise to carry out the ideas in the production of nuclear energy with the motivation of making nuclear energy sustainable, safe, and economically viable. SCCME, Service of Corrosion and Materials behavior in their Environment, employs over 60 scientists and technicians, and 15 Ph.D. students and post-docs. Within SCCME, LM2T principal topic concerns the corrosion of materials in extreme environmental conditions and carry out both experimental and theoretical studies. LM2T is dedicated to the Thermodynamics and Thermochemistry Modelling of materials via atomistic and thermodynamic simulations/calculations. LM2T is world-renowned for their CALPHAD expertise.

The experimental and theoretical tools available in LM2T are:

- CALPHAD modeling skills to access the phase diagrams of many metallic and oxide complex systems for high temperature material applications;
- an *in-house* Advanced Temperature and Thermodynamic Investigation by Laser Heating Approach facility (ATTILHA) to obtain new experimental data

Subject:

To aid in understanding the high temperature interactions in oxide of SiO_2-B_2O_3-Na_2O (SBN) melts and slags, a thermodynamic approach is retained. The Post-Doctoral candidate will be responsible for building up the SiO_2-B_2O_3-Na_2O (SBN) CALPHAD database and implementing the extensions to amorphous systems. For that, the Gibbs energy functions for all phases as a function of the chemical composition, temperature, and pressure will be assessed to build a database from which the equilibrium can be calculated by minimization of the total Gibbs energy of the system.

Up to now the phases of SiO_2-B_2O_3-Na_2O (SBN) liquids, extending to glasses, are outside of the current scope of the CALPHAD databases. In the frame of this work, attemps to develop specific models (two state model) for amorphous systems will be performed.

Furthermore, the acquisition of new experimental data will be performed using the in-house **A**dvanced **T**emperature and **T**hermodynamic **I**nvestigation by **L**aser **H**eating **A**pproach (ATTILHA) facility to provide phase diagram data for the thermodynamic assessment. Some millimetric samples will be prepared to make suitable demixed samples with the aid of the ATTILHA facility. After preparation, samples will undergo some basic preliminary tests to acquire some of their physical properties (SEM observations, XPS analyses).