

Annual Report 2010

GLASS STRUCTURE (TC03)

Composition of the TC03 Technical Committee:

Chair: Francisco Muñoz Fraile (Ceramics and Glass Institute, Spain)
Vice-chair: Akira Takada (Asahi Glass, Japan)
Members: Joe Zwanziger (Dalhousie University, Canada)
Adrian C. Wright (Reading University, U.K.)
Natalia Vedishcheva (Institute Silicate Chemistry, Russia)
Ondrej Gedeon (Institute of Chemical Technol., Czech Republic)
Doris Ehrh (Otto-Schott Institute, Germany)
Liu Qiming (Wuhan University of Technology, China)
Hiromichi Takebe (Ehime University, Japan)
Efstratios Kamitsos (Nat. Hellenic Research Foundation, Greece)
Laurence Galois (IMPMC CNRS 7590, France)
Lionel Montagne (Lille University, France)
Alex Hannon, (Rutherford Appleton Laboratory, U.K.)

SUMMARY

2010 has been a transition year for TC03. Josef Zwanziger has been the interim Chair of TC03 since 2009 until September 2010. However, in order to carry out new TC03 commission, Francisco Muñoz Fraile (Spain) and Akira Takada (Japan) were appointed as the new Chair and Vice-chair, respectively, after the last International Congress on Glass held in Brazil during September.

Due to the quite broad scope of topics covered by the former TC03 (Basic Glass Science) and, as a consequence of the recent formation in 2009 of 3 new TCs focused on computer modelling, structure and vibrations and structure-properties relationships, the Technical Committee TC03 has changed its objectives to a group mainly devoted to the study of the structure of glasses. Thus, TC03 has been renamed **Glass Structure**.

Approximately half of the members (before September 2010) have shown their availability to continue collaboration within new TC03 objective. New members have also been contacted to ask for their participation and they accepted to be involved. They are Lionel Montagne (University of Lille, France), Laurence Galois (IMPMC CNRS 7590, France) and Alex Hannon (Rutherford Appleton Laboratory, UK).

ACTIVITIES IN 2010

Meetings

There have not been formal meetings of TC03 members during 2010. However, informal discussions were held during the 11th International Conference on the Structure of Non-Crystalline Materials (Paris, France) and the International Congress on Glass (Salvador, Brazil) by the few members present in either of

the conferences, in order to solve the organisational issues and define the new working lines for the near future.

NMR Round Robin Test

Samples of four sodium borosilicate glasses, which composition and properties can be found in reference [“Electrical conductivity and viscosity of borosilicate glasses and melts”, D. Ehrt and R. Keding, *Physics and Chemistry of Glasses*, 50(3), (2009), 165-171] and were prepared by Doris Ehrt in the Otto-Schott Institute (Jena, Germany), were distributed to several Laboratories for NMR characterisation. Table 1 shows that nominal composition of the studied glasses.

Table 1. Composition of investigated NBS glasses.

| Samples | Na ₂ O (mol %) | B ₂ O ₃ (mol %) | SiO ₂ (mol %) |
|---------|---------------------------|---------------------------------------|--------------------------|
| NBS-A-1 | 12.5 | 62.5 | 25 |
| NBS-B-2 | 3 | 48.5 | 48.5 |
| NBS-C-3 | 15 | 42.5 | 42.5 |
| NBS-D-4 | 6.5 | 33.5 | 60 |

The Professors/Researchers in charge of this test were: Scott Kroeker (University of Manitoba, Canada), Randy Youngman (Corning, USA), Pierre Florian (CNRS, France), Mark Smith (University of Warwick, UK) as well as Josef Zwanziger (Dalhousie University, Canada). Results are complete from Zwanziger and Kroeker; reports are being completed by Youngman and Florian and measurements are underway at several other labs. While data have been collected on various aspects, one representative graph, of four-fold-coordinate boron fraction N_4 , is shown in Figure 1.

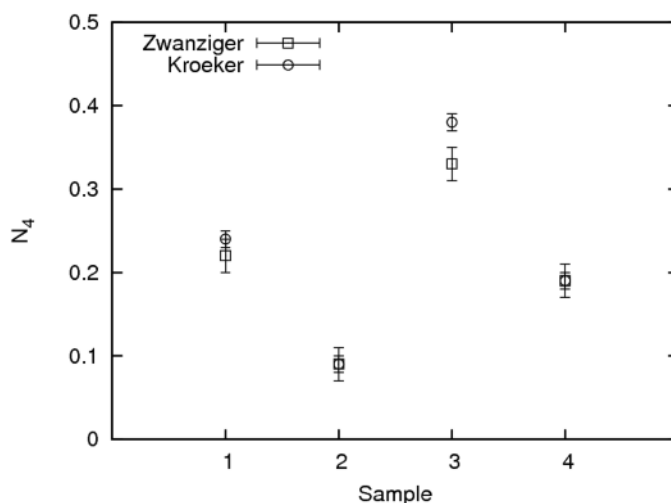


Figure 1. N_4 values in NBS glasses.

In conjunction with the round robin test, Natalia Vedishcheva estimated the fractions of basic structural units, densities and Q^n values successfully by employing the modelling of the chemical structure.

Symposium

Adrian Wright, Natalia Vedishcheva and Josef Zwanziger, from TC03, together with Edgar D. Zanotto of TC07, organised for the **ICG 2010 Conference** a session on the **Structural Basis of Glass Crystallisation** where an invited talk and five more papers were presented. Both technical committees affirmed the success of collaborative discussions and the continual exchange of discussion after this symposium.

Education

During a stay at the University of Trento (Italy) through invitation of Giuseppe Dalba, Adrian Wright presented a 6-lecture course on "**X-Ray and Neutron Amorphography**".

PLANS FOR 2011

In order to continue the work of TC03 within the topic of Glass Structure, it has been decided to keep running the activities planned in the former Basic Glass Science committee that would best fit in the new organised one. Thus, the main objectives to be carried out during 2011 are the following:

Round-robin test

Once all results of the Round Robin Test on the four samples of $\text{Na}_2\text{O-B}_2\text{O}_3\text{-SiO}_2$ glasses can be completed, an analysis of the influence of the NMR experimental parameters on the speciation of the borate and silicate structural units will be carried out.

All four borosilicate glasses present subliquidus phase separation. It has been discussed that, meanwhile it would be more suitable for a start to perform a characterisation based on a single-phase homogeneous glass sample, it will be quite interesting to standardise and complete the structural characterisation in the sodium borosilicate glasses that is already running by the mentioned laboratories.

As more laboratories continue to join the TC03 committee, the round robin test will be extended to other potential characterisation techniques that could better fulfil the gaps that Nuclear Magnetic Resonance could not achieve by itself. This will be a chance to properly combine NMR with diffraction techniques, for example.

Computer modelling of glass structure

The previous activities in TC03 were to perform a "round robin" test to evaluate the various computer simulation codes currently used to investigate the vitreous states. However, in order to cooperate more with the experimental round-robin tests, the objective will be changed. First, the present state of advanced NMR

simulation will be investigated. If the techniques have applicability they will be evaluated using round-robin results. Second, results of atomistic modelling will be compared with those of the chemical structure modelling.

NMR round robin test results on the structure of the borosilicate glasses under study will also be used in comparison with the modelling of the chemical structure through a purely thermodynamic model of associated solutions, a model developed by N. Vedishcheva and coworkers [more information: ref. N.M. Vedishcheva *et al.*, J. Non-Cryst. Solids 345&346 (2004) 39-44].

Glass microstructure

It has been proposed that the subject under study of TC03 might be extended to Glass Microstructure and the relationship between atomic structure and phase separation behaviour.

Education

This objective was first established to act in collaboration with TC23 in the improvement of students' training, from a general point of view related to Glass Science, and as a consequence of the fact that not very adequate students' training might be occurring. Despite future collaboration with TC23 within this subject, the intention is that a series of workshops/seminars can be planned with the topic "Glass Structure", not only for students but also for glass researchers in general, who would need to specialise in structural characterization techniques of glasses.

Meeting and symposium

At the moment, a TC03 meeting is planned for 2011 in Oxford (UK) within the framework of the **International Conference on the Chemistry of Glasses and Glass forming Melts** in celebration of the 300th anniversary of the birth of Mikhail Vasilievich Lomonosov. At the same place, a session on the **Chemical Aspects of Glass Structure** will be organised by the members of TC03.