13th ICG SUMMER SCHOOL

GLASS FORMATION, STRUCTURE, AND PROPERTIES

Energetics, Environment and Glass Manufacturing

28th June – 2nd July 2022 - Berlin, Germany

Scientific Program

BASIC SCIENCE

	Tuesday	Wednesday	Thursday	Friday	Saturday
08h30	Introduction to the Course/ICG (JP)				
08h45	Optical absorption and redox chemistry. (**J. Parker**)	Structure (I): Neutron and X-ray diffraction (**R. Vacher**)	Mechanical properties of glass (I) **R. Hand**	Modelling (I): atomistic simulations (**A. Takada**)	Student presentation of projects
09h45	Thermodynamics of glasses I: One-component and multicomponent oxide glasses (**R. Conradt**)	NMR in oxide glasses (I) (**P. Florian**)	Glass ceramics (I): Sintered glass ceramics and glass matrix composites (**R. Mueller**)	Vibrations (I): basics of IR absorption, Brillouin and Raman scattering. **(B. Hehlen**)	Student presentation of projects
10h45	**Coffee break**	**Coffee break**	**Coffee break**	**Coffee break**	10h15 **Coffee break**
11h00	Mass transport in glass. (**J. Parker**)	Structure (II): Neutron and X-ray diffraction: applications (**R.Vacher**)	Mechanical properties of glass (II) **R. Hand**	Modelling (II): Bridging between macroscopic and microscopic phenomena (**A. Takada**)	Student presentation of projects
12h00	Thermodynamics of glasses II: Example: Chemical Durability (**R. Conradt**)	NMR in oxide glasses (II) (**P. Florian**)	Glass ceramics (II): Thermal analysis (**R. Mueller**)	Vibrations (II): relation with glass structure (**B. Hehlen**)	12h **Closing**
13h00	**Lunch**	**Lunch**	**Lunch**	**Lunch**	
14h30	Students describe their own research activities (5 min /person).	Project allocation & start work on project	Tutorials (see list)	Tutorial (see list)	
15h30			Project workshops	Project workshops	
18h00	Title to be announced (E. Muijsenberg)			Title to be announced (C. Claireaux)	
19h00	**Welcome reception**			**School Dinner**	

TUTORIALS

Glass and phase diagrams - quantitative treatment of multicomponent systems: assessment of glass properties (thermal, mechanical, chemical), approach to structural features & approach to the energetics of glass melting - How to identify the positions of complex glasses in phase diagrams.

Calculating Raman activities : activity of the Raman modes in crystals for a given symmetry and scattering geometry - Molecular selection rules of simple liquids - the case of glasses.

Diffusion coefficient: Values of D, examples. Activation energies. Balance of D *vs* stress relaxation in ion exchange toughening: Optimum temperature range. Significance of $(Dt)^{1/2}$. Examples of time and distance *e.g.* tin bath depth, chemical toughening, chemical durability effects at room T. Crystal growth, nucleation, coarsening.

Practical aspects on atomistic simulations: how to calculate atomic structures and mechanical, transport and optical properties by simulations.

LIST OF LECTURERS

C. Claireaux	CelSian glass & solar BV	Eindhoven - Netherland	*corinne.claireaux@celsian.nl*
R. Conradt	Aachen University & uniglassAC GmbH Co.	Aachen - Germany	*reinhard.conradt@gmail.com*
P. Florian	CEMHTI-CNRS	Orleans - France	*pierre.florian@cnrs-orleans.fr*
R. Hand	University of Sheffield	Sheffield - UK	*r.hand@sheffield.ac.uk*
B. Hehlen	University of Montpellier	Montpellier - France	*bernard.hehlen@umontpellier.fr*
R. Mueller	Bundesanstalt für Materialprüfung und -forschung (BAM)	Berlin - Germany	*ralf.mueller@bam.de*
E. Muijsenberg	Glass service sa	Vsetin - Czech republic	*erik.muijsenberg@gsl.cz*
J. Parker	University of Sheffield	Sheffield - UK	*j.m.parker@sheffield.ac.uk*
A. Takada	Univeristy College London (ex-AGC)	Tokyo - Japan	*akira_takada_scientist@yahoo.co.jp*
R. Vacher	Université de Montpellier -CNRS	Montpellier - France	*rené.vacher@umontpellier.fr*

ABSTRACTS

&

BIOMETRICS

LABORATOIRE CHARLES COULOMB MONTPELLIER

Reinhard Conradt

Professor
Consultant through own company uniglassAC GmbH,
Aachen - Germany

Bio :

Reinhard Conradt is a retired professor from RWTH Aachen University, Germany. He has been performing glass research at Fraunhofer Institute of Silicate Science, ISC Würzburg, Germany, for six years, then served for ten years as university lecturer and industry consultant at Chulalongkorn University, Thailand. From 1997-2016, he was full professor and Chair of Glass & Ceramic Composites at RWTH Aachen University, Germany. His work has been committed to building bridges between science, especially chemistry, thermodynamics and kinetics, and industrial engineering. This comprises fundamental research as well as the evaluation and optimization of industrial processes. Presently, he is serving as president of the International Commission on Glass ICG.

Abstract:

Glasses are typically perceived as amorphous materials lacking any translational order at the atomic scale. They show, however, a distinct short- and medium-range order (corresponding to the nature of coordination polyhedra and their mutual linkage, respectively). From the point of view of energetics, glasses of a given composition differ from their crystalline counterparts by a small enthalpy and entropy difference only; at temperatures above 298 K, they show nearly the same density of (non-dissipating!) vibrational states (DVS). As a consequence, they behave like elastic solids, and may thus be treated like low-density polymorphs of the given composition. This concept applies to one- as well as to multi-component systems. It forms the basis for a concise thermodynamic description of solid glasses and their melts. The advantage of this approach consists in a quantitative description of all glass properties based on DVS, like: heat capacities, heats of formation, elastic properties, as well as a quantitative description of processes where a glass or its melt is involved as a reaction partner. In a ***first lecture***, the concept is presented and underpinned with practical examples. This involves the evaluation of known phase diagrams. The extension to industrial problems requires a further step, i.e., the identification of phase equilibria in systems with truly many components. In a ***second lecture***, the concept is applied to the field of glass corrosion in aqueous media. It is shown how the hydrolytic stabilities of glasses are correctly predicted from their chemical composition.

Pierre Florian

Research Ingineer,
Conditions Extrêmes et Matériaux : Haute Température et Irradiation (CEMHTI) - CNRS
Orléans - France

Bio:

Pierre Florian is a specialist of Solid-State Nuclear Magnetic Resonance (SSNMR) spectroscopy. His research focuses on the application of the state-of-the-art SSNMR methods to material science and in particular to the characterization of structural and/or chemical disorder. He also has a long standing experience in very-high temperature NMR, up to 2400°C.

He currently holds a position of site manager at the CEMHTI laboratory (CNRS Orléans, France), handling a group of 3 engineers and 6 spectrometers including two very high fields (750 and 850 MHz) part of the french NMR delocalize infrastructure IR-RMN THC for which he is the local contact in charge of a total of more than 300 days of access per year on the NMR platform.

Abstract:

NMR in silicate glasses

We will first briefly recall the basic principles of Nuclear Magnetic Resonance spectroscopy, using a classical formalism. The specificity of this technic when applied to Solid-State will then be exposed, emphasizing the experimental conditions required, the known issues such as sensitivity and the description of two-dimensional NMR.

In a second part, we will illustrate the type of information that can be recovered from NMR in the case of glassy materials. Examples will be given from studies performed on oxides, silicates, alumino-silicates and phosphates glasses. In the course of this overview, various one- as well as two-dimensional technics will be presented along with their use to quantify the short- and medium-range chemical and structural disorder present in glasses.

Russell J Hand

Professor of Glass Science & Engineering
University of Sheffield, UK
Past-President of the Society of
Glass Technology, UK

Bio:

Russell Hand obtained his first degree and PhD in Physics from the University of Cambridge. After a 1 year Post-Doc in Cambridge he moved to the now Department of Materials Science and Engineering, at the University of Sheffield in 1989, as the Redland Research Fellow. He was appointed to a Lectureship in 1990 (Senior Lecturer 2001; Reader 2010; Professor 2012) and in 1999 obtained an MEd in Teaching and Learning for University Lecturers. His research interests are focussed on the mechanical properties of glasses, radioactive waste vitrification and the durability and vitrified wasteforms. Between 2014-2017 Russell was President of the Society of Glass Technology. He is Secretary of the Coordinating Technical Committee of the ICG and is also a member of Technical Committees 5 (Waste Vitrification), 6 (Mechanical and Nanomechanical Properties of Glass), 23 (Education) and 28 (Glass Fibres).

Abstract:

Mechanical properties of glasses I

Many glasses are well known as brittle materials with low fracture toughnesses that are flaw sensitive. This has implications for both how we measure the mechanical properties of glasses and also in how we attempt to modify those properties, whether through residual stresses, coatings or even compositional variation. In this first lecture I will concentrate on examining on what we can measure, what has to be taken into consideration in making those measurements, and what those measurements reveal to us. Thus material properties such as toughness, hardness and modulus will be considered along with specimen properties such as strength.

Mechanical properties of glasses II

In the second lecture I will start by considering the flaws that control the strength of glass, how they arise and their distribution. The effects of environmental interactions will also be considered. I will then move on to examine the techniques we can use to improve the mechanical performance of glasses the use of residual stresses introduced by thermal or chemical means as well as the use of coatings.

Bernard Hehlen

Professor
Department of Physics
University Montpellier - France

Bio:

Pr. Dr. Bernard Hehlen (51) obtained a doctoral degree (Ph.D) from the University of Montpellier in 1995. His Ph.D work, initiated by K.A. Müller (Nobel laureate 1987), concerned the possibility of a novel coherent quantum state in the prototypical ferroelectric system $SrTiO_3$. He obtained an EC grant for a post-doctoral fellowship position in Oxford (UK) at the Clarendon Laboratory. He had to resign his contract in 1996 when he got a position of teacher and researcher at the 'Laboratory of Glasses' in Montpellier. He became Professor in Physics in 2004. His scientific activity concentrates on the structural and vibrational properties of disordered systems, including glasses, ferroelectrics and relaxor materials. He is an experimentalist, working on neutron and X-Ray scattering at large facilities and light scattering experiments.
He was member of the scientific board of the 'inelastic- scattering' group at the neutron scattering center in Grenoble (ILL, 2000-2004). Between 2007 and 2013 he was heading a regional platform gathering Brillouin, Raman, hyper-Raman, and Infrared absorption spectrometers. He is currently chairman of TC26 'Vibrations and Glass Structure' at the International Commission on Glass (ICG), coordinator of the cluster "Basic Science", and member of the TC23 'Education'. From 2005 to 2014 he was responsible of a Master degree in 'condensed matter Physics' then "Nanophysics" at the University of Montpellier.
His scientific achievements have been published in 56 articles in peer-revue journals and books, and give rise to 59 oral communications including 18 on invitation by the organization committee. In 2004 he has been laureate of the Gottardi prize awarded by the ICG, for the construction of a hyper-Raman scattering spectrometer devoted to the study of glasses.

Abstract:

Atomic vibrations in glasses: basics & relations to glass structure

An introduction to the linear response theory will allow first to define the concepts of susceptibility, fluctuation spectra, auto-correlation functions, etc., and to link these quantities to the experimental data through the fluctuation-dissipation theorem. In a second step, we will treat the origin of the light scattering giving rise to the Raman and Brillouin selection rules. The latter will be exploited to relate the experimental observations to the local and medium range structure of oxide glasses taken in the family of silicates, borates and aluminosilicates.

John Parker

Emeritus Professor
Department of Material Science and Engineering
University of Sheffield - UK

Bio:

Emeritus Professor Parker began his University Education at the University of Cambridge in 1964 where he studied for 8 years, obtaining an MA in Natural Sciences, a PhD in Earth Sciences and 2 years post-doctoral experience. From there he moved to the University of Sheffield to teach Glass Technology (1971-2009). His teaching and research interests have covered a wide spectrum but specifically have included optical fibres, dental cements, defects in glass making, structure and optical absorption. Although now formally retired he still teaches in Sheffield. He is also heavily involved in the Society of Glass Technology and in ICG, particularly its Coordinating Technical Committee, Web site, and Winter/Summer Schools. He writes a monthly article for Glass International on History of Glass Making and is Curator of the Turner Museum of Glass, giving frequent talks on the collection, its history and art.

Abstract:

Transport properties

Diffusion underpins the kinetics of many glass making processes. This talk will look at mathematical descriptions of diffusion and how experimental results can be obtained and interpreted. We will also examine the factors affecting diffusion coefficients and what happens when more than one species is mobile. Finally we will examine in greater depth ion exchange processes used in generating toughened glasses and optical waveguides.

Colour and redox processes

This talk will give an overview of the generation and control of colour in glass, including measurement techniques. The effect of the interaction between active ions and the local structural environment will be considered. Many of the transition metal ions used in colouring glass have more than one oxidation state and the importance of redox reactions in glass making will be stressed.

Akira Takada

Visiting Professor
Department of Earth Sciences
University College London - UK
and
Department of Science and Engineering
Ehime University - Japan

Bio:

After graduating from Tokyo University at which I studied applied mathematics, I joined Asahi Glass Company. I have been performing a variety of computer simulations of macroscopic and microscopic phenomena on glass. My recent major concern is to construct a bridge between microscopic (glass structure) and microscopic phenomena (glass properties) on glass. I am joining the activities of TC-3 (Glass Structure) and TC-27 (Atomistic modelling and Simulation) under ICG. In addition, I have a research project at University College London as a visiting professor.I served as a president at the Japan Society of Industrial and Applied Mathematics (JSAM; a number of member is about 1,700) in 2013-2015. I am a member of Science Council of Japan. I am Fellow of JSIAM and Fellow of SGT (Society of Glass Technology).

Abstract:

Bridging between macroscopic and microscopic phenomena

For the former half of career, I undertook the task of modeling macroscopic phenomena such as heat exchanger, glass melt flow and vico-elastic deformation of glass. In those days no commercial software codes were available and I had to develop my own codes. Appropriate mathematical modelling is essential, however, it is also important to presume appropriate initial and boundary conditions as well as material properties for simulation. More challenging aspect is that material properties are non-linearly depenant on chemical conposition, temperature profile and etc.
.For the latter half of my career, I have devoted to microscopic phenomena in order to design glass materials. Microscopic simulation techniques such as molecular dynamics simulation and ab initio simulation have well-founded theories, but only small space-scale and short time-scale behaviors of material can be tackled with due to the requirement of a huge computation time. Several approaches to bride between macroscopic and microscopic phenomena are discussed in my lecture.I believe numerical modeling will contribute to discover wonderful treasure islands in the field of glass science and technology!

René Vacher

Emeritus Professor
Department of Physics
University Montpellier - France

Bio:

René Vacher was born in 1943. He is Emeritus Director of Research at the French « Centre National de la Recherche Scientifique (CNRS) ». He has been working in the field of Physics of glasses for more than 40 years. His main research activities concern the structure, the vibrational dynamics, and the elastic properties of glasses. He is also well known for his contributions to the Brillouin spectroscopy of light in solids, to the inelastic neutron spectroscopy of glasses, and to the structure and dynamics of aerogels.

He is (co-)author of 150 papers in journals with peer review and chapters in books, and 70 articles in conference proceedings. He has directed 15 PhD. Students.

He was director of the « Laboratory of glasses » in Montpellier, France, from 1982 to 1998, Head of Physics department from 1999 to 2002 at the University of Montpellier. From 1992 to 1999, he was director of the CNRS « Groupement de Recherche Physique des Verres ».

He was chairman of the conference « Glass Odyssey », annual meeting of the International Commission of Glasses (ICG) in 2002 and of the « Third European Conference on Neutron Scattering » in 2003, in Montpellier. He chaired the scientific committee of the Internal Congress on Glass held in 2007 in Strasbourg, France. From 2009 to 2016, he was chairman of the Coordinating Technical Committee of the International Commission on Glass.