MechGlass2024
USTVerre Thematic Day
January 12, 2023

Paris, France
Institut de Physique du Globe de Paris (IPGP)
Cover: (left) DCDC (double cleavage drilled compression) glass sample with a symmetric crack growing in the sample. (right) Half a DCDC glass sample after it has been broken into 2 revealing the fracture surfaces. ©C. L. Rountree
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Introduction

Glass is an everyday material, which humanity has used since the Stone Ages and fabricated since well before the Common Era. Today its uses range from cookware in our kitchens to lenses in outer space and high-tech components. The wide use of glasses is due to numerous advantageous properties, including transparency, high stiffness and hardness, low thermal expansion, high melting point, relative inertness, etc., yet despite these numerous advantageous properties glass still has a major drawback: It is fragile. Industry has tackled this issue via several schemes: altering the chemical composition, invoking phase separation, layering glass, replacing Na+ ions by K+ ions, etc. This thematic day will look at current issues concerning the mechanical properties of glasses with special emphases on:

- Plasticity
- Fracture across time and length scales
- Micromechanics
- Issues concerning industrial applications (including microelectronics)
- Emerging issues (including 3D printing)
- ...

This thematic day will set up a work plan for a Mechanics of Glasses summer school.

Organizing committee

Etienne BARTHEL  Sciences et Ingénierie de la Matière Molle
Daniel BONAMY  Service de Physique de l’Etat Condensé
Laure CHOMAT  Service de Physique de l’Etat Condensé
Jean-Pierre GUIN  Institut de physique de Rennes
Daniel R. NEUVILLE  Institut de Physique du Globe de Paris
Cindy L. ROUNTREE  Service de Physique de l’Etat Condensé
Maxime VASSAUX  Institut de physique de Rennes

Language

The primary language of MechGlass2024 is French; however, participants are welcome to present in either French or English.
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<td>Cindy L. ROUNTREE</td>
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<td>CEA</td>
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<td>Université de Montpellier</td>
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<td>Jean-Pierre GUIN¹ &amp; Etienne BARTHEL²</td>
<td>Université de Rennes &amp; ESPCI</td>
<td>Dureté, plasticité - une approche de la résistance à la fissuration des verres silicatés</td>
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<td>CEA, CNRS</td>
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Oxide glasses have many advantageous properties, including optical transparency, low thermal expansion coefficients, thermally insulating, etc. As such, they have a number of applications in the world today (windows in buildings, dishes, protection panels for plasma screens and solar panels, etc.). However, one major drawback is they are brittle. In general, stresses applied at the boundaries of a glass sample concentrate around a crack front as a function of $K\sqrt{r}$, where $r$ is the distance from the crack front and $K$ is the stress intensity factor. In a vacuum, for a crack to propagate the stress intensity factor ($K$) is greater than fracture toughness ($K_c$, a material parameter). It should be noted that the $\frac{1}{\sqrt{r}}$ tendency breaks down very near a crack front in the zone coined the process zone. In real life, atmospheric conditions are relevant. Glasses, which seem to fail abruptly, frequently fail due to the growth of a slowly evolving crack front which progresses from slow growth to dynamic growth. When considering the slow growth of a flaw, the crack fronts velocity depends on environmental parameters (e.g. temperature and humidity). This slow growth is coined stress corrosion cracking. There are actually the four zones of sub-critical crack propagation:

- Region 0: presents a threshold limit for $K_I$ below which the crack front velocity ceases to propagate. The region is also coined the environmental limit, $K_e$.
- Region I: the crack velocity is set by the rate of the stress enhanced chemical reaction between water molecules and stretched chemical bonds in the OGs.
- Regime II: the crack velocity is limited by the transport of water molecules to the crack tip.
- Regime III: the velocity raises sharply with $K_I$.

Beyond environmental parameters, the regions also depend on the chemical composition of the glasses. This presentation will first present the process zone size in pure silica [1]. Then, it will consider how the chemical composition of $\text{SiO}_2-\text{B}_2\text{O}_3-\text{Na}_2\text{O}$ glasses alters the fracture response of the glasses [2-3].

**SiO₂ behaviour in direct bonding mechanism**

*Frank FOURNEL*

**CEA-LETI**

Direct bonding has evolved into a well-established technique facilitating various 3D applications. Silicon dioxide to silicon dioxide hydrophilic direct bonding is currently in mass production within microelectronic foundries. Nevertheless, ongoing studies are still being conducted on the hydrophilic direct bonding mechanism.

The behavior of silica at the bonding interface holds significant interest for comprehending adhesion and adherence development in this unique case. It will be demonstrated that silica hydrolysis with water plays a pivotal role. Additionally, measuring direct bonding energy using the anhydrous DCB technique will provide insights into the silica fracture mechanism. Notably, the fracture does not appear to be fragile, and a viscoplasticity behavior is required to elucidate the bonding energy measurement involving the silica layer.

More recently, the introduction of a minuscule amount (1/100 of a monolayer) of specific molecules (such as DEAE or NaOH) has significantly enhanced adherence for low post bonding annealing temperature. These molecules seem to catalyze silica hydrolysis, reinforcing its crucial role in the direct bonding mechanism.

**Reducing glass carbon footprint – The other reduction levers**

*René GY*

**Saint-Gobain Recherche**

Glass industry globally emits almost 100 Mt CO₂ each year. The new Oräé® float glass shows that by increasing cullet in the batch and using more of green energies, the float glass CO₂ emission can be reduced by 42%. Other promising developments are currently underway at the melting step to go even further. In this talk we overview the potential of other levers like finding more sustainable alternative materials for glass, glass light weighting and glass reuse. Insulation, reinforcement, glazing, and packaging applications are considered. Some mechanical issues are pointed out.
Dynamic fracture of alkali silicate glasses: insights from large scale atomistic simulations

Simona ISPAS

Laboratoire Charles Coulomb (L2C), Université de Montpellier/CNRS

The fracture of oxide glasses is a subject of high complexity since many factors (e.g. length scale under investigation, strain rate, chemical composition, etc…) play an important role. Using large scale molecular dynamics simulations, we have investigated the composition dependence on the fracture behaviour of sodium silicate glasses on the microscopic scales. While silica glass presents a nearly perfect brittle fracture behaviour, we have found that the one of sodium rich glasses is accompanied by the nucleation of irregular voids as large as 3-4nm ahead of the crack front, indicating the presence of nanoductility for these glasses. We have also explored the spatial and temporal changes of various atomic-level properties and the correlations between them. It has been found that these properties are spatially very heterogeneous with disorder becoming more pronounced for alkali rich compositions. Close to the crack tip, a heating of several hundred degrees above the average temperature has been identified, which permits the structure to relax.
Room temperature viscoplastic response of amorphous olivine films revealed by advanced ex-situ and in-situ TEM nanomechanical testing

**Hosni IDRISSI**

Institute of Mechanics, Materials and Civil Engineering (IMMC), UCLouvain, B-1348, Louvain-la-Neuve, Belgium

Olivine is a silicate which controls the rheology of the Earth’s mantle down to ca. 410 km depth. Recently, we have discovered a new deformation mechanism of olivine where grain boundary sliding involves amorphization of grain boundaries under high stresses and further plastic flow along this amorphous layer [1]. We are convinced that this mechanism has a fairly general application to hard materials under conditions of high stress. This idea has been advocated by Idrissi et al. in [2]. In the present case of olivine, the implications are mainly in the lithosphere in a ductile brittle context and at the boundary between the lithosphere and the asthenosphere. This led us to characterize the mechanical properties of amorphous olivine, but this material is mostly available in the form of thin films. It is therefore necessary to employ nanomechanical techniques: nanoindentation, in-situ TEM deformation and Lab-on-Chip. These tests have in particular the capacity to extend the solicitations to very low deformation rates relevant in geodynamics. Advanced TEM characterizations have allowed to identify the underlying microscopic mechanisms either in-situ or in ex-situ deformed samples. These data will allow in the future to feed mesoscopic mechanical models of olivine-rich rocks of the upper mantle. We also observe a significant influence of the electron beam on the viscoplastic behaviour of amorphous olivine. Special attention was paid to elucidate the origin of such feature.

**References**


Combining predictive analytics with scientific research to streamline time to develop High Performance Glass Fiber composites for wind energy.

Anne BERTHEREAU
Owens Corning

Wind energy is currently one of the leading growth platform for High Performance Glass fibers with blade lengths reaching up to 107 and even 115 meters for Global Wind OEM. To enable for that always longer & stiffer blades, glass fiber products for windmill blade have to fulfill a complex set of customers specifications, two of them being modulus and fatigue performances. While modulus is directly correlated to glass composition, extensive literature studies showed that the glass-size-resin interphase has a high impact on the composite fatigue performance. Here, predictive analytics gives Owens Corning an edge in materials development. It is today possible to correlate the viscoelastic properties of composites interface and fatigue composite performance and so to build predictive models. A project will be presented which is a good example of the power of combining traditional empirical approach and new data science predictive approach to develop high performance materials. It enables Owens Corning to reduce the time it takes to test composites materials from weeks to hours.

Additive manufacturing of glasses

Ronan LEBULLENGER
Rennes Institute of Chemical Sciences (ISCR - UMR CNRS 6226), Université de Rennes

An overview of the different methods of additive manufacturing of glasses will be presented. The pros and cons will be detailed. Some examples of recent developments in FFF (Fused Filament fabrication) and SLS/M (Selective laser sintering/melting) in Rennes will illustrate the use of 3D printing for biomaterials and IR applications.

Dureté, plasticité - une approche de la résistance à la fissuration des verres silicatés

Jean-Pierre GUIN\textsuperscript{1} et Etienne BARTHEL\textsuperscript{2},

\textsuperscript{1} Institut de Physique de Rennes (IPR), Université de Rennes
\textsuperscript{2} ESPCI

La génération de fissures par indentation est très couramment utilisée pour qualifier la résistance mécanique des verres silicatés. Nous présenterons une brève review de la littérature puis nous introduirons les approches micromécaniques développées recemment pour mettre en relation réponse plastique locale et fissuration.
Etude du comportement des verres sous impacts hypervéloces

Didier LOISON

Institut de Physique de Rennes (IPR), Université de Rennes

Dans le domaine spatial comme dans les installations laser de haute puissance, les matériaux utilisés dans la conception des systèmes et de leurs diagnostics sont sollicités dans des conditions extrêmes. En ce qui concerne les impacts hypervéloces dus aux collisions entre des débris volants à plusieurs km/s et les systèmes opérationnels, il est nécessaire d’étudier le comportement des matériaux utilisés dans cette gamme de sollicitation (pression allant jusqu’à plusieurs Mbar et vitesse de déformation autour des 107 s⁻¹).

Ainsi, l’équipe dynamique, choc, impact de l’IPR et ses partenaires étudient depuis 10 ans le comportement de deux familles de verres dans ces conditions de chargement :

- Les verres d’oxydes utilisés pour leur transparence dans les hublots et diverses optiques (achromat, lentille, lame de phase, ...) utilisés dans les diagnostics scientifiques des installations laser et des équipements embarqués sur les navettes, satellites et stations spatiales.

- Les verres métalliques présentant un potentiel intéressant en tant qu’élément de blindage afin d’améliorer les boucliers espacés (Whipple Shield) actuellement utilisés sur la station spatiale internationale.

Pour générer ce type de sollicitation, nous générions des chocs grâce à des impulsion laser, les diagnostics résolus en temps renseignent sur les états thermodynamiques de la matière et sur l’évolution de l’organisation atomique.
Estimation du seuil de fissuration à l'aide de modèles à gradient d'endommagement : application aux matériaux vitrocéramiques sous auto-irradiation

Gérald FEUGUEUR1,2, Lionel GÉLÉBART1, Corrado MAURINI2, Sandrine MIRO3

1 Université Paris-Saclay, CEA, Service de Recherche en Matériaux et procédés Avancés, 91191, Gif-sur-Yvette, France
2 CNRS, Institut Jean Le Rond d’Alembert, Sorbonne Université, UMR 7190, Paris, France
3 CEA, DES, ISEC, DE2D, Université de Montpellier, Marcoule 30207, France

Les verres actuellement utilisés pour le confinement des déchets nucléaires peuvent incorporer un taux de charge en produits de fission et actinides mineurs allant jusqu’à 18,5% massiques. Les matériaux vitrocéramiques envisagés pour cette application seraient une alternative intéressante qui permettrait de diminuer le volume de colis en augmentant ce taux de charge. Cependant, pendant le stockage, les inclusions de phases cristallines, riches en produits de fission, seraient soumises à une auto-irradiation α provoquant un gonflement susceptible d’engendrer une fissuration de la matrice vitreuse [1].

Les méthodes FFT, sont particulièrement adaptées à la simulation du comportement mécanique de matériaux hétérogènes. En effet, comparés à l’utilisation de codes Élément-Finis « standards », les codes FFT sont souvent bien plus performants et très bien adaptés à une implémentation parallèle en mémoire distribuée. Initialement proposée pour des modèles de comportement locaux, linéaires ou non-linéaires, l’utilisation de ces méthodes s’étend désormais au cadre des modèles non-locaux, tels que l’endommagement à gradient [2]. Par ailleurs, pour simuler la fissuration, les modèles à gradient d’endommagement [3], [4] font l’objet d’un intérêt croissant dans la communauté mécanicienne. Cette formulation permet de prédire non seulement la nucléation de fissures, mais aussi la propagation de ces dernières. Malheureusement, le choix des paramètres du modèle \((G_c, l_0)\) pour reproduire à la fois les conditions d’amorçage et de propagation s’avère délicat. En effet, ce choix est limité par la taille des hétérogénéités mais aussi par la résolution du support de calcul. La solution qui a été envisagée dans le cadre de cette application consiste à choisir une longueur interne \(l_0\) raisonnable vis-à-vis de la discrétisation spatiale et d’adapter \(G_c\) afin de respecter un critère d’amorçage fixé par les « essais » [5]. L’implémentation du modèle de « champ de phase » proposé par Bourdin et al. [4] a été mis en place au sein de codes FFT [2] et notamment au sein du code massivement parallèle AMITEX_FFTP. La résolution du problème sans hypothèses simplificatrices (approche en champ complet) s’avère généralement très coûteuse et des approches simplifiées reposant sur l’hypothèse d’un champ d’endommagement homogène par phase ont été mises en place récemment dans AMITEX_FFTP.

Une première partie sera consacrée à la présentation des différentes approches et des méthodes pour estimer le seuil de nucléation des premières fissures. Les différentes approches seront ensuite confrontées dans un second temps par des simulations FFT dans le cadre d’une étude portant sur l’effet de la distance entre 2 inclusions en 2D après avoir déterminé plusieurs jeux de paramètres du modèle \((G_c, l_0)\). Enfin, des analyses seront présentées sur des cellules avec une distribution aléatoire d’inclusions (Figure 1) en utilisant les outils génériques développés au CEA tel que Combs et Voxelize pour la génération de ces microstructures.

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Useful Information

Talks will be held at the Amphithéâtre, IPGP of Institut de Physique du Globe de Paris (IPGP) located at 1 Rue Jussieu, 75005 Paris. It is situated on the ground floor to the left of the main entrance.

Coffee breaks will be offered in the main entrance hall.