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CeRTEV - Center for Research, Technology and Education in Vitreous Materials

Report 6 January – June 2019

Edgar Dutra Zanotto Hellmut Eckert Ana C.M. Rodrigues Karina Lupetti Eduardo B. Ferreira

RESEARCH PROGRESS

1. Fundamental Aspects of Glass Crystallization

CeRTEV advances in the area of glass crystallization have involved both theoretical concepts and new experimental monitoring approaches. On the theoretical side improvements to the classical nucleation theory (CNT) have been proposed [1] and an important comparison with Molecular Dynamics Simulations has been conducted on a model system [2]. Experimental progress comprises new monitoring results of stoichiometric [3] and non-stoichiometric [4] and an improved understanding of the role of nucleation agents [5].

1.1. Theoretical Advances

To achieve a quantitative agreement of experimental data with theoretical predictions, in classical nucleation theory a curvature- or size-dependence of the surface tension of critical clusters has to be accounted for. For its description, frequently the Tolman equation is chosen. Tolman derived his relation originally in application to droplets or bubbles in one-component fluids assuming that nucleation is caused by variations of pressure. As shown in our recent work his approach and the resulting basic relations are applicable also to the description of crystal nucleation in multi-component fluids if either pressure or temperature is changed. Estimates of the Tolman parameter in application to crystallization are advanced for both the mentioned cases. The Tolman parameter is shown to depend on the surface tension for a planar interface, the number of

components in the liquid, the bulk properties of both the liquid and crystal phases, and the way the metastable state is generated. In addition, we develop a method of improving the precision in the specification of the curvature dependence of the surface tension in melt crystallization going beyond the Tolman equation in its original form. The results are applied successfully to the description of crystal nucleation in silicate glass-forming melts [1].

Fundamental insights into homogeneous nucleation and growth were obtained via Molecular Dynamics simulation on the model system of liquid supercooled BaS, using a recently developed two-body interatomic potential on 36,000 particles. Isothermalisobaric MD simulations were done at three temperatures. The calculated pair correlation function, along with several snapshots, allowed us to quantify the nucleation times, their crystal growth rates, and the time evolution of overall crystallization. Nucleation was spontaneously achieved in the supercooled liquid state, allowing the average onset time of the first nucleus to be calculated for 15 samples over a range of temperatures temperature. In this way the steady-state nucleation rates, MD Jss (T) were determined. Independently, the MD results allowed determinations of the diffusion coefficients, D (T), the melting point, Tm, and the enthalpy of melting, Δ Hm. Based on these results, the MD Jss could be compared with the predictions of the Classical Nucleation Theory (CNT) for homogeneous nucleation using the nucleus/liquid interfacial free energy, σ , as the sole fitting parameter. The calculated critical nucleus is made of only 2 to 3-unit cells, which is consistent with the critical size observed in the simulations, approximately 10-15 atoms. Using a constant (fitted value of) σ and the D (T) and thermodynamic parameters from the simulations, the MD pre-exponential factor turns out to have the same order of magnitude as the theoretical value predicted by the CNT. Such (rarely-reported) agreement of the predictions of CNT and MD simulations supports the validity of the CNT for simple supercooled liquids [2].

1.2. Experimental Investigations

1.2.1 Monitoring stoichiometric and non-stoichiometric crystallization

Crystallization of barium disilicate supercooled liquid, an important model system studied previously by us via vibrational spectroscopy and MD simulations, presents multiple exothermic events that were carefully monitored by stepped differential scanning spectroscopy accompanied by XRD analysis. The first exothermic event involves crystallization of H-BaSi2O5 (monoclinic), and Ba₃Si₅O₁₃, however, both L-BaSi2O5

(orthorhombic) and an unknown phase are also formed. The second exothermic event involves the transformation of H-BaSi₂O₅ into L-BaSi₂O₅, in addition to the formation of further unidentified crystalline material. These results clarify the relationships between thermal history and crystalline phase formation, which may be used to produce tailored glass-ceramics [3]. In general, all the properties of glass-ceramics are strongly dependent upon their nano- or microstructure, including the percentage, composition and, structure of the residual glass phase. Unfortunately, however, determining the chemical composition of the residual glassy phase is far from trivial and there are very few publications on this matter. A new approach is the use of electrical conductivity measurements by impedance spectroscopy to infer the composition of the residual glass in partially crystallized Li₂SiO₃-CaSiO₃ glasses [4]. The glass-ceramics were obtained by heat-treatment at 560°C for distinct periods, in conditions where only lithium-metasilicate (Li2SiO₃) crystallized. Consequently, residual glasses of the resulting glass-ceramics became depleted in lithium, and their ionic conductivity and the respective activation energies changed accordingly. Therefore, the compositions of residual glasses can be inferred by comparing the glass-ceramics ionic conductivities and activation energies with those of reference glasses having known chemical compositions. This approach was additionally validated by Tg measurements using differential scanning calorimetry. The electrical conductivity measurements have the distinct advantage of being nondestructive and allowing the crystallization process to be followed in situ [4].

1.2.2. Volume nucleation effected by nucleation agents

Diopside-based ceramics and glass–ceramics ($25CaO \cdot 25MgO \cdot 50SiO_2$) have been studied because of their applications in electronics and biomedicine. As diopside glass presents poor internal nucleation ability, the corresponding glass-ceramics are usually obtained via sintering surface crystallization of sintered glass powders. To avoid this process, the use of nucleating agents has been explored. Using Fe₂O₃ nanoparticles we were able to induce copious internal nucleation in this glass, which enabled the production of single-phase diopside glass–ceramics by the traditional route. The crystallization kinetics of a sample containing 8.26 mol% of Fe₂O₃ was investigated under isothermal conditions by differential thermal analysis (DTA) and was modeled by the Johnson-Mehl-Avrami-Kolmogorov-Erofeev (JMAKE) equation. The mechanism and kinetics of crystallization of the iron-diopside formed (Ca₀.991(Mg₀.641Fe₀.342)(Si₁.6Fe₀.417)O₆) were elucidated by DTA, which provided relevant information to guide the development of this novel type of internally crystallized glass-ceramic [5].

2. Strong Glasses and Glass-Ceramics

2.1. Engineered stones are promising materials for kitchen countertops, floor and facade tiles and other application in construction. They consist of approximately 70–95 wt% of mineral particles (usually quartz) dispersed in a matrix made of cement, ceramics, or, much more often, polymer resins. Despite their very attractive aesthetic appeal, polymer matrices entail low wear resistance, low chemical resistance and degradation by UV radiation or elevated temperatures. To overcome these drawbacks, new composites were developed based on recycled window glass containing up to 70% weight of albite, alumina, petalite or quartz and characterized with respect to their flexural strength, hardness, water absorption, thermal shock resistance and chemical durability. Except for the quartz/glass composites, low-porosity materials (<10%) with competitive properties if compared to commercial products were obtained. For instance, an alumina/glass composite showed a (4-point) flexural strength of approximately 115 MPa and a hardness of 9 GPa. The petalite/glass composite exhibited high thermal shock resistance $(\Delta T_c \sim 330^{\circ}C)$; whereas the albite/glass composite showed excellent chemical stability against concentrated acids and bases [6].

2.2 Ultrastrong glasses with high crack resistance are of great interest for the optimization of low-weight flat displays in modern handheld electronic devices. In this context intense development efforts are devoted to new oxide glass formulations for improving the mechanical strengths without compromising other physical properties. An important issue in this regard has been the conflicting demand of hardness and crack resistance upon the glass composition. The beneficial effect of magnesium oxide upon the performance of crack resistant oxide glasses has been explored in a series of aluminoborosilicate glasses with the compositions $60SiO_2-(20-x)Al_2O_3-xB_2O_3-20Na_2O$ and $60SiO_2-(20-x)Al_2O_3-xB_2O_3-10Na_2O-10MgO$. The simultaneous presence of both boron and aluminum oxides in these glasses produces a synergetic effect upon the crack resistance, whose structural origins were explored by detailed ¹¹B, ²³Na, ²⁷Al, and ²⁹Si single and double resonance solid state NMR studies. The Mg-driven enhancement of crack resistance in Na-Mg boroaluminosilicate glasses in comparison to analogous Mg-free glasses can be related to a reduction in the fraction of four-coordinate boron (N₄), producing higher concentrations of non-bridging oxygen species. For boron-rich glasses

(x = 20, 15, 10), this trend is accompanied by the expected decrease in E-modulus. For low-boron glasses, however, the reduction of E-modulus owing to the decrease in N₄ is over-compensated by the strong interaction of the non-bridging oxygen species with the high-field strength cation Mg²⁺. Finally, in the boron-free aluminosilicate endmember series, the formation of higher-coordinated aluminum contributes to a *simultaneous* increase in both crack resistance and E-modulus [7].

3. Bioactive glasses and glass-ceramics

3.1. Biosilicate functionalization for extended applications

Monolithic and powdered Biosilicate® glass-ceramics have been widely recognized as excellent materials for bone tissue engineering applications. In vitro, in vivo, and clinical studies - including histopathological cytotoxicity, and genotoxicity analyses - over the past 25 years have proven the tremendous potential of this material for applications in the form of osteoinductive powders, scaffolds and even monolithic pieces. CeRTEV's effort during the past few years have focused on the development of new formulations and processing methods for widening the application spectrum of Biosilicate. Specific progress achieved during the past 6 months is highlighted below.

3.1.1. Highly porous Biosilicate® glass-ceramics have been obtained in the form of 3D printed scaffolds and foams, using an alternative processing route, based on the thermal treatment of silicone polymers containing micro-sized oxide fillers. This processing method helps to improve the integration between materials synthesis and shaping. The products show regular geometries, large open porosity (~60 vol%) and high compressive strength (~7 MPa). Open-cellular foams with porosity up to ~80 vol% were also prepared from liquid silicones mixed with several fillers, including hydrated sodium phosphate. This specific filler acts both as a foaming agent (release of H₂O) and as a provider of liquid phase upon firing in air at $1000^{\circ}C$ [8].

3.1.2. New antibacterially active bioactive glass-ceramics of the SiO_2 –CaO–Na₂O–P₂O₅ system have been developed by doping with up to 3 mol% of Ag, Mg, Sr, Zn, and Ga. Their antibacterial activity was confirmed against 23 oral bacteria, related to caries and endodontic infections. The lowest minimum inhibitory concentration (MIC) values were found for Ag-doping, for which no viable cells were observed after 24 h incubation in the biofilm-forming capability assay. Direct contact assays confirm a significant reduction in the number of viable cells after only 10 min in contact with the microorganisms. This result indicates that the tested materials have an intrinsic

antibacterial activity, stimulating future studies involving their application as topical endodontic disinfectants or in dental prophylaxis procedures [9].

3.1.3. Antibiomicrobial fuctionalization of Biosilicate has also been of great current interest beyond the dental application field. In this connection the structural consequences of incorporating boron have been studied by ¹¹B MAS NMR of both glassy and crystallized specimens. Boron is found to be present in the form of three-coordinate pyroborate units, with only minor fractions of four-coordinate species while ³¹P MAS-NMR spectra reveal that phosphorus is almost exclusively present in the form of orthophosphate. The demand of the anionic borate network former for cationic charge compensation leads to an increase in average connectivity of the silicate network, as evident from ²⁹Si MAS NMR. ³¹P/¹¹B dipolar recoupling experiments indicate negligible amounts of borate-phosphate linkages in these glasses. Crystallization produces NaCaPO₄ and Na₂CaSi₂O₆ as well as a residual amorphous material for which the fraction of four-coordinate boron is significantly increased [10].

3.1.4. Other Developments

Finally, in the relatively new application area of bioactive glasses and glassceramics in the field of orbital implants for ocular surgery, new opportunities arise from the release of angiogenic and antibacterial agents, helping to improve anophthalmic socket procedures. Existing orbital implants based on bioactive glasses have been reviewed and the further potential and open challenges for future research in this field are highlighted and discussed [11].

3.2. Bioactive lithium silicate ceramics

Glass-ceramics based on the Li₂O-SiO₂ system have been extensively used as restorative dental materials due to their excellent chemical durability, aesthetics, inertness in the buccal environment, and high fracture strength; but they are not bioactive. On the other hand, all known bioactive glasses show ability to bond to bone, teeth and cartilage coupled to osteoconduction and osteoinduction, but their fracture strength and toughness are rather low. Promising multi-component systems have been developed o impart bioactivity on lithia-silica glass ceramics based on both lithium metasilicate (LM) and lithium disilicate (LD). Neither ceramic was shown to be cytotoxic, and lithium ion release for LD was found to be outside the toxic range (>8.3 ppm). LD shows good cellular adhesion and proliferation, leading to the formation of a mineralized matrix after 21 days [12].

4. Glasses and Glass-Ceramics for Energy Technology Applications

4.1. NASICON-based glasses and glass-ceramics from the Na_{1+x}Al_xGe_{2-x}(PO₄)₃ system were synthesized for $0 \le x \le 1.0$. As observed in previous Li-based systems, conductivities increase and activation energies decrease with increasing Al content, x. This effect may be rationalized by both the increase mobile ion concentration and the increase in the unit cell volume of the NASICON structure [13].

4.2. Network former mixing effects in ion conducting oxyfluoride glasses with compositions xWO_3 -30NaPO₃-(70-x)NaF, with $30 \le x \le 70$ were studied and discussed in relation to bulk physical properties and structural features. As the NaF content increases, the glass transition temperature decreases systematically, indicating a successive depolymerization of the glass framework. NMR and Raman studies indeed confirm that NaF acts like a network modifier resulting in the formation of W-F bonds via breakage of W-O-W and W-O-P linkages [14].

5. Photonic Glasses and Glass-Ceramics

5.1. Glass matrices for light converters, scintillators and white light generation

An important part of the CeRTEV agenda is the further development of new rareearth doped glass matrices for scintillators, white-light generation, and other applications involving UV-to-visible or infrared-to-visible light conversion. During the past reporting period detailed studies have focused on the compositional development and photophysical properties of new glass systems showing promise for these applications:

5.1.1. Nd-doped oxyfluoro tellurite glasses and glass-ceramics with chemical composition TeO₂-ZnO-YF₃-NaF (TZYN) were prepared and their luminescence was analyzed via Judd-Ofelt theory [15]. Glass-ceramics obtained by controlled heat treatment of the glasses at 390°C for 5 h contain homogeneously dispersed nano-crystalline NaYF4:Nd with lifetime values of the 4F3/2 excited state lifetime (187 μ s) significantly higher than the glasses (124 μ s) [15]. These materials are promising candidates for enhanced solar light harvesting in photovoltaic cells by converting UV and IR radiation to visible (where the absorption of Si cells is more effective) and thus improving overall efficiency of photovoltaic cells.

5.1.2. Dy₂O₃ doped calcium boroaluminate (CaBAI) glasses with composition $50B2O_3$ -(25-x) CaO-15A₁₂O₃-10CaF₂-(xDy2O₃) (x = 0.0, 0.5, 1, 2, 3, and 5 wt%) were

studied as new materials for white light emission. Photoluminescence spectra measured under 405nm excitation are characterized by the $4F9/2 \rightarrow 6H15/2$ (blue) and $4F9/2 \rightarrow 6H13/2$ (yellow) transitions. The yellow/blue intensity ratio depends on Dy₂O3 doping level. The simulation of a combination of a Blue LED (BL) emission with the sample emission was studied in the CIE diagram, indicating the suitability of these materials for smart white light generation [16].

5.1.3. Fluorophosphate glass and glass-ceramic compositions doped with Eu_3+ , Tb_3+ and Dy_3+ for scintillating devices. For the past year, new fluorophosphate compositions based in the system NaPO₃-Ba(PO₃)₂-MgF₂-YF₃ doped with Eu, Tb and Dy trivalent ions have been developed for the purpose of high energy (UV, X-ray) sensitization and conversion to visible light. This process is known as scintillation and it is an important application since exposure to high energy radiation can cause severe damage to biological tissue. The aim of the studies is to develop prototypes of compact sensors for UV and X-ray radiation.

5.2. Photonically or electronically altered optical materials

5.2.1. Photo-thermo-refractive (PTR) glass is an optically transparent photosensitive Na₂O-ZnO-Al₂O₃-SiO₂ glass, containing NaF and KBr additives, along with cerium, silver, tin, and antimony oxide dopants. After heating above 500 °C, UVexposed regions of this glass produce permanent refractive index changes, presumed to be associated with the precipitation of NaF nanocrystals. In a first application of solid state NMR to this technologically important system, the short- and medium-range order of this glass system have been studied using multinuclear single- and double-resonance solid-state NMR spectroscopy. The results have been compared with those obtained in various model glasses with simplified compositions. The NaF component is shown to modify the aluminosilicate framework, producing of F-bonded five- and six-coordinated aluminum species. The detailed fluoride speciation was deduced from ¹⁹F MAS-NMR spectra, supported by ${}^{19}F{}^{27}Al$ and ${}^{19}F{}^{23}Na$ dipolar recoupling experiments. The majority of fluoride within the PTR glass is found within Na-dominated local environments, which also interact strongly with the aluminum. ²³Na{¹⁹F} rotational echo double resonance reveals that about 1/3 of the Na⁺ ions have fluoride ions in their first coordination spheres [17].

5.2.2. Further CeRTEV activities in this area during the past reporting period involve the use of EPR and optical spectroscopies to monitor redox processes upon

radiation exposure and other aging processes. While these studies are still in progress, some preliminary results can be summarized as follows:

(1) For glasses in the system NaPO₃-Sb2O₃-CuO, EPR results show that increasing contents of Sb₂O₃ lead to successive reduction of Cu₂+ to Cu+, which suggests the oxidation of Sb₃+ to Sb₅+ [18],

(2) Lithium diborate and sodium diborate glasses can be used for gamma-ray dosimetry, by monitoring the defects generated via UV-Vis spectroscopy [19],

(3) EPR in combination with luminescence spectroscopy is suitable for monitoring aging processes in ceramic YPO4-powders in Xe excimer lamps [20].

(4) Silver- containing fluorophosphate glasses may be successfully altered by femtosecond laser irradiation, producing tailorable three-dimensional fluorescent microstructures that contain silver nanoclusters and nanoparticles with different spectroscopic properties [21].

5.3. Inorganic-Organic Luminescent Hybrid Systems

Organometallic complexes based on the transition metals Ir, Pt, Os, Cu, etc are largely studied for their high triplet luminescence efficiency that can yield several applications. In the search for understanding and improving the luminescence of optical materials based on Ir(III) complexes, 3 $[Ir(C\sim N)_2(dnbp)]^+$ (dnbp = 4,4'-dinonyl-2,2'-bipyridine) the emitters were immobilized in MCM-41 mesoporous nanoparticles. By taking advantage of the amphiphilic nature of $[Ir(C\sim N)_2(dnbp)]^+$, the complexes were mixed with an appropriate surfactant and the resulting micelles served as templates for the synthesis of mesoporous SiO₂ host materials in a 1-step sol-gel route. The MCM-encapsulated $[Ir(CN)_2(dnbp)]^+$ complexes present intense emissions with prominent rigidochromic spectral changes that are substantially less affected by O₂ as compared to methanolic solutions, with a thousand-fold decrease in quenching rate constants. Host-guest systems of this kind may become suitable for future optoelectronic devices, rigidity optical sensors, or biological markers in different colors [22].

Rhodamine 6G-doped TEOS-derived xerogels containing different concentrations of TiO₂ nanoparticles with average diameter of about 350 nm were designed to study random laser action. The volumetric distribution of the TiO₂ particles was shown to have a great impact upon the random laser energy threshold and emission spectra. These results suggest that the way scatterers are volumetrically distributed can increase or decrease the pump energy required for laser action [23]. 6. References (CeRTEV faculty in yellow)

[1] Schmelzer, J.W.P., Abyzov, A.S., Ferreira, E.B., Fokin, V.M., International Journal of Applied Glass Science 10 (2019), 57-68.

[2] Prado, S.C.C., Rino, J.P., Zanotto, E.D. Computational Materials Science 161 (2019), 99-106.

[3] Moulton, B. J. A.; Rodrigues, A. M.; Sampaio, D. V.; Silva, L. D.; Cunha, T. R.; Zanotto, E. D.; Pizani, P. S. Crystal Engineering Communications 21 (2019), 2768-2778.

[4]_Nuernberg, R.B._Bello, T.S.,_Fokin, V.M., Zanotto, E.D., Rodrigues, A.C.M. Journal of Non-Crystalline Solids 510, 15 (2019), 158-165.

[5] Mastelaro, V.R., Bayer, P.S., Zanotto, E.D., Journal of Materials Science 2019, in press.

[6] Santos, G.G., Crovace, M.C., Zanotto, E.D. Composites Part B: EngineeringVolume 167 (2019) 556-565.

[7] Bradtmüller, H.; Uesbeck, T.; Eckert, H.; Murata, T. T.; Nakane, S.; Yamazaki, H.; Journal of Physical Chemistry C 2019, in press.

[8] Elsayed, H. Rebesan, P., Crovace, M.C., Zanotto, E.D., Colombo, P., Bernardo, E. Journal of the American Ceramic Society 102 (2019), 1010-1020.

[9] Siqueira, R.L.; Alves, P.F.S., da Silva Moraes, T., Casemiro, L.A., da Silva,
 S.N., Peitl, O., Martins, C.H.G., Zanotto, E.D. Ceramics International 45 (2019), 9231 9244

[10] Bradtmueller, H.; Cerrutti, B. M.; Souza, M. T.; Zanotto, E. D.; Eckert, H., Journal of Non-Crystalline Solids 505 (2019), 390-399.

[11] Baino, F.Verné, E., Fiume, E., Peitl, O., Zanotto, E.D., Brandão, S.M., Schellini, S.A., International Journal of Applied Ceramic Technology 2019, in press.

[12] Daguano, J.K.M.B., Milesi, M.T.B., Rodas, A.C.D., Weber, A.F. Sarkis, J.E.S., Hortellani, M.A., Zanotto, E.D.: Materials Science and Engineering C 94 (2019), 117-125.

[13] Ortiz-Mosquera, J.F., Nieto-Muñoz, A.M., Rodrigues, A.C.M. Journal of Non-Crystalline Solids 513 (2019), 36-43.

[14] Munhoz, J. F. V. L.; Santagneli, S, H.; de Oliveira, M. Jr.; Rodrigues, A. C.
 M.; Eckert, H.; Nalin, M., Journal of Non-Crystalline Solids 505 (2019), 379-389.

[15] Rajesh, D.[,] de Camargo, A.S.S., Journal of Luminescence 207 (2019) 469-476 [16] Lodi, T.A. Dantas, N.F.,Gonçalves, T.S., de Camargo, A.S.S., Pedrochi, F., Steimacher, A., Journal of Luminescence 207 (2019), 378-385.

[17] Funke, L. M.; Janka, O.; Poettgen, R.; Glebov, L.; Hansen, M. R.; Eckert, H.,J. Phys. Chem. C 123 (2019), 12411-12422.

[18] Franco, D.F. Carvajal, E.E., Donoso, J.P., Silva, M.A.P., Sant'Ana, A.C., Fares, H., Magon, C.J., Nalin, M. Journal of Non-Crystalline Solids 503-504 (2019) 169-175.

[19] de Oliveira, L.N., do Nascimento, E.O., Andreeta, M.R.B., Antonio, P.L., Caldas, L.V.E. Radiation Physics and Chemistry155 (2019), 133-137.

[20] Broxtermann, M.; Funke, L. M.; Keil, J. N.; Eckert, H.; Hansen, M. R.;
Meijerink, A.; Yu, T.; Braun, N.; Jüstel, A T. Journal of Luminescence, 202 (2018), 450-460.

[21] de Castro, T.; Fares, H.; Khalil, A.A.;Laberdesque, R.; Pwetit, Y.; Strutinski,
C.; Danto, S.; Jubera, V.; Ribeiro, S. J. L.; Nalin, M.; Cardinal, T.; Caniopni, L. Journal of Non-Crystalline Solids 517 (2019), 51-56.

[22] Zanoni, K. P. S.; Vilela, R. R. C.; Silva, I. D. A.; Murakami Iha, N. Y.; Eckert,
H.; de Camargo, A. S. S., Inorganic Chemistry 58 (2019), 4962-4971.

[23] Sciuti, L.F., Gonçalves, T.S., Tomazio, N.B., de Camargo, A.S.S., Mendonça, C.R., De Boni, L., Journal of Materials Science: Materials in Electronics 2019, in press

EDUCATION AND OUTREACH

Ana CM Rodrigues (Coordinator) Karina Lupetti (Researcher)

<u>Group A:</u> Development of professional qualification strategies in glass science and technology

The course "Technician in Glass Production", a project in partnership with the Paula Souza Center, Abividro and the glass company Nadir Figueiredo, started with its first cohort in February 2018. At the present date, June 2019, the first group of 40 students are in the process of completing their third and final semester and will be submitting their course completion work (in Portuguese, Trabalho de Conclusão de Curso- TCC) soon. We already know that some of them will be hired by the Brazilian company Nadir Figueiredo. Further follow-up regarding their professional development will be done after the students will have received their degrees (July 2019).

During this semester, faculty training for this course was still continuing, with three programs:

- April $12^{th} - 13^{th}$ - 16 hrs – covering the themes "*Glass Furnaces*" held at Paula Souza Center, SP

- May 10th - 11th - 16 hrs *Structure*, properties and processing of refractories for glass industry, held at LaMaV/UFSCar

- July 25th to 26th: visit to ACG – float glass plant (Guaratinguetá, São Paulo state) and a glass transformer.

The second cohort of students in the Centro Paula Souza at Mogi das Cruzes will start in August 2019. The public selection procedure had more than 3 candidates per vacancy, which is considered very good for Centro Paula Souza. We are looking forward to welcoming these new students and to accompany their progress.

A second unit of our partner Centro Paulo Souza has also expressed an interest in offering the course *Technician in Glass Production*. This unit of the Centro Paula Souza is located in São Bernardo do Campo, near the Brazilian glass industry "Wheaton", which mainly produces glass bottles for the cosmetics industry. We do believe that the opening of this course in São Bernardo do Campo will assist the development of the glass industry in the region, and CeRTEV is looking forward to assisting the introduction of this course in a second unit of the Centro Paula Souza.

EduSCar:

In November 2018, a network named *EduSCar* (Education for São Carlos) was created involving 5 CEPID programs and authorities linked to São Paulo State governmental institutions for education management. In the two last months of 2018 and first months of 2019, there were several meetings of this group, aiming to present a common project to FAPESP and other funding institutions.

EduSCar is an initiative of coordinators and professors who develop large projects in the public universities of São Carlos, SP. Within these projects, these professors and researchers have the mission of interacting with the educational systems of their cities, engaging in scientific dissemination and promoting scientific education. This joint initiative has full support of and integration with the Teaching Board and the Municipal Department of Education, so that we can involve all the schools in São Carlos in complementary activities, aiming at training and supporting teachers in the education of science, portuguese language and mathematics. The main goal of EduSCar is to promote an increase in the overall performance of <u>high school</u> students from approximately 50 public schools in São Carlos and contribute to a leverage of their better education. Results from this initiative will be evaluated from the evolution of grades by already existing learning assessment systems.

The Research Centers linked to FAPESP and CNPq already promote numerous activities in Dissemination and Popularization of Sciences, which include: Science Clubs, Science fairs, Ludo Educativo, Education spaces, with the participation of students and teachers from public schools, various courses on informatics, teacher training, educational TV, internet classes (e-classes), creation and donation of educational kits to schools, among others. The integration of all these activities, through the joint action of the groups forming EduSCar, will certainly produce synergistic effects, helping to promote the teaching agenda of São Carlos public schools in a more professional and forceful way. If our actions turn out to be measurably successful, our aim is to extend those activities towards the national level.

Group B: Diffusion of basic and glass science

Educare vacations (January 21st-25th) involving 25 children per day

The Educare vacation happens every January and brings together not only but mainly children from the neighborhood "Samambaia" community in São Carlos. It aims to provide vacation activity for these children, with the prospect of presenting educational topics related to science.

During the period January 2019, the theme *Water* was addressed as a topic of fundamental importance for the environment and life on Earth. There were various workshops with 2 hours of duration. Activities included sewing a drop of water made of felt tissue; with the study of polyacrylamide beads, which are transparent in water; planting of succulents, watercolor, scientific theater, cooking, biscuit sculpture, slime and demonstration of sculptures in vegetables. There was also a walk on the Samambaia trail and the presentation of the theater piece "*Science that Laughs*: *where is my water?*" The activities took place at "Espaço Educare" and had 5 monitors and 5 teachers from different arts / science workshops.

Theater performances:

During the period January to June 2019, 5 different theater pieces were presented for 500 attendants at events in São Carlos, as described in the following:

January, 22st: "Science that laughs: where is my water" (Educare vacation) - 40 spectators.

<u>Synopsis:</u> Scientist Kryptonia and her cousin Xenonio show the importance of water and dialogue with the children to find solutions to save this precious possession.

February 2nd: "*Science that laughs: glass world*" (EVQ UFSCar) - 150 spectators Scientist Kryptonia and her cousin Xenonio speak of the different types of glass and the daily life of scientific discoveries.

April, 13st: "Petit Curie" (Tech Novation ICMC) - 250 spectators

The story of Marie Curie is told through an interactive and inclusive shadow theater with the "Olhares" group.

May 8th: "A New Sense" (Cecília Meireles College) - 40 spectators

A play for sensitization is experienced by the students of the 1st year of high school of the Cecília Meireles College in São Carlos.

May 11th: "Lucis est vita" (Educare, Mother's Day) - 20 spectators

A play that speaks of light in the eyes of those who do not see. The *Olhares* group is presented to the public that participates in the activity of Mother's Day in the "Educare Space". This presentation is part of the celebrations of the 10 years of Grupo *Olha*res.

Vitreous Sounds

The musical group continues the presentations by invitation of different events.

New musical instruments of glass are being studied and created.

March 8th: Women's Day- 20 spectators

March 13th: UFSCar Community Library- reception of the freshmen- 30 spectators

May 11th: Educare Mother's Day - 30 spectators

June 7th: Premiere of "*L'AQUA*", in the 2nd Week of Environmental Engineering - UFSCar Campus "Lagoa do Sino"- 150 spectators (<u>https://www.youtube.com/watch?v=rtTDRn5-TgI&t=32s</u>)

Workshops

February 13th: 1st Workshop on *Molecular Gastronomy - Senses and Flavors* (3 hours) at the 39th Summer School in Chemistry UFSCar - 40 participants

February 13th: 1st Workshop on *Scientific Theater* (3 hours) at the 39th Summer School of Chemistry UFSCar 6 people

March 12th: 1st Workshop Experiments *and World of glass*; 2 hours (reception of freshmen of Chemistry Department, UFSCar) - 50 participants.

May 18th: 1st Workshop on *Molecular Gastronomy - Confectionery* (3 hours) (PET ECOSOL) - 20 participants

5 Workshops *Science in the kitchen* at UAC (Unidade de Atendimento à Criança , or Child Care Unit, UFSCar), for four-year-old children, total of 10 hours. 15 participants / day

The themes of gastronomy and senses were addressed, thinking about the inclusion of children with visual and intellectual disabilities, as well as vegans and vegetarians. The children cooked and tasted different flavors of fruits, legumes and vegetables. There were 5 meetings that happened in the classroom that became an improvised kitchen to follow the recipes that we proposed during the semester.

June 18th - Lecture "Senses and Flavors" - Day of Chemistry, Institute of Chemistry, IQ-UNESP Araraquara- 60 participants

Glass Museum in the Ventura Space

Every day, the Ventura Space Glass Museum welcomes visitors who appreciate its exhibits. Two exhibitions are now in the locales: "Science and Inclusive Art" and "Art in Glass". The visitors who come to this space are among undergraduate students, graduate students and professors from different institutions who are delighted to learn about glass science and glass art. In this semester, more than 100 visitors have already visited the glass museum in the Ventura Space.

Organization of the Pint of Science São Carlos (May 20-22) 100-300 participants / day

CeRTEV helped in the organization of *The Pint of Science* in São Carlos. In this year, this well-known event addressed several subjects, among them: mathematics, periodic table, data science and paleontology. There were an average audience of 100 to 300 people per night in each of the 3 bars in which the Pint of Science happened this year.

Vitreous Minute:

Since 2016, 72 narratives of the *Vitreous Minute* have been created, broadcast weekly by Radio UFSCar 95.3 FM. Podcasts present the science and curiosities about vitreous materials in a language appropriate to the general public.

In 2019, 15 new *Vitreous Minutes* were created, which are part of the project of Scientific Journalism IV, by the scholar Karina Omuro Lupetti.

Other Activities

Mangas (Glass Comics Stories)

Our four volumes of Glass Stories Comics, in the Japanese style "Manga" were translated to English. This translation was funded by the International Commission on Glass and the comics were presented at the 25th International Congress on Glass, held in Boston, June 2019. The TC 23 (Technical Commission 23, on Glass Education) of the International Commission on Glass is currently discussing about a policy on how those comics could be printed and distributed in English-speaking countries

More than 800 illustrations of the glass stories that the children created in schools of the municipal public network were digitized, whose narratives are in the process of being recorded in partnership with *Rádio UFSCar*. Thirty stories were created and will be published in October 2019.

<u>Videos</u> for the project *Basement of Science*

Five new videos of the *Glass* series were created: "*Candies: Edible glasses*", "*Glasses singing: Glasses and acoustics*", "*Glass shielded: Glasses resistant*", "*Glasses colored and glasses that change color*" and "*Optical fiber*".

Publication

The book chapter "Science, Art and Scientific Lettering: an analysis of collective narratives and illustrations / comics on glasses " by Adriana Yumi Iwata and Karina Omuro Lupetti, was accepted to compose the seventh volume of the collection: "Natural Sciences and Teacher Training" organized by Wender Faleiro, Alessandra Aparecida Viveiro and Maria Paulina de Assis, with prospects of publication in the 2019.

INNOVATION AND TECH TRANSFER REPORT

Eduardo Bellini Ferreira – EESC / USP (Coordinator) Edgar Dutra Zanotto – DEMa /UFSCar Oscar Peitl – DEMa /UFSCar Sergio Luis da Silva – UFSCar (Tech Transfer Manager)

As we have stressed before, we pursue new technologies in all the main fields of CeRTEV's main plan and their transfer to the productive sector. We base our strategy on three pillars: i) establishment of cooperation agreements and licensing of on-demand technologies commissioned by industry, focusing the skills of our group to bring the industry close to our academic institutions, connecting universities, companies, and other institutions through cooperation programs as PITE and PPP/FAPESP, and FINEP; ii) nucleation of spin-off companies from the group activities, stimulating entrepreneurship, and encouraging engagement in programs such as PIPE/FAPESP; and iii) extensive promotion of innovation and technology transfer, accomplished by our extensive knowhow in these subject areas combined with the assistance of agencies at UFSCar (www.inovacao.ufscar.br) and USP (www.inovacao.usp.br). We list below the activities related to our Innovation and Tech-transfer effort ("science to business approach") to channel the CeRTEV's research achievements into innovation.

Establishment of cooperation agreements and licensing of on-demand technologies commissioned by industry in this period

<u>E. D. Zanotto</u> has carried out various consultancy services for companies, namely, **Guardian**: melting behavior of SLS glasses with different types do dolomite, **Vimaster**: characterization of glass microspheres; **AGP**: Specification and norms for testing armor glasses for vehicles, and **Vetra**: melting, XRF, FTIR and DSC characterization of F18 bioglass; and signed an one-year contract on special glass-ceramics with **AGC**, Japan (76,000 \in) starting on Aug/2019.

<u>E.D. Zanotto</u> chaired up to April/2019 the Scientific Council of the *Instituto Serrapilheira*, the first private research foundation within Brazil, and managed a research project funded by this Institute, which finished in March 2019.

On March/2019, <u>A.C.M. Rodrigues</u> met with A.F.Y.T. Imada Technology R&D Engineer, **Nadir Figueiredo**, Mogi das Cruzes/SP, to discuss and negotiate a proposal on the analysis of coatings in glass; under analysis.

<u>O. Peitl</u> carried out consultancy services for **Schott Flat Glass do Brasil** on the problem of tempering and staining on the silkscreen of glasses.

<u>H. Eckert</u> has an ongoing project with the **Nippon Electric Glass** company on the structure-property relations for crack-resistant glasses; and signed an NDA with **Schott Glass Company** on structural characterization of fluorophosphate glasses.

<u>M.R.B. Andreeta</u> has an ongoing project with the company Alacer Biomédica (R\$ 173.250) Nov/2017-Nov/2019 on *Development of solid-state pH sensors*, a systematic study on the preparation of new vitreous and glass-ceramic systems based on borosilicates as solid-state pH sensors. <u>M.R.B. Andreeta</u> is also negotiating a PIPE/FAPESP with the Brazillian company Engecer.

Further actions for the establishment of cooperation agreements will be considered according to the research advances made in each area.

Nucleation of spin-off companies from the group activities

VETRA High-Tech Ceramic Products, a CeRTEV spin-off company, established in São Carlos in August 2014 to offer glass and GC biomaterials combining unique features such as biodegradability, bioactivity and bactericidal action, is advancing. The company has actively participated in outreach activities promoted by CeRTEV and collaborated in pre-clinical and clinical research with several departments from various universities (Unicamp, Unifesp, Unesp, USP). Two projects were recently submitted to FAPESP in collaboration with the Department of Medicine at the University of São Paulo and another PIPE project exploring new technology. The patent BR 10 2017 01064 "*Implant for volume reposition in anophthalmic cavities in humans or animal, process for obtaining it, device for implant machining and its use*" was also licensed by VETRA and this product is being analyzed by the Brazilian Health Regulatory Agency (Anvisa). Vetra also submitted two other products to Anvisa and is tightening ties and closing supply contracts with two national companies.

Extensive promotion of innovation and technology transfer

Patent filed in the Brazilian National Institute of Industrial Property (INPI)

<u>M. Nalin</u> filed the patent 17AUIN080 "*Product and process for the preparation of oxide glasses and optical fibers for use in faraday rotators*" (in Portuguese): March/2019, in the Brazilian National Institute of Industrial Property (INPI) as results of the scientific and technological efforts of his team in a field of interest of our CEPID. The

analysis at INPI, unfortunately, may take from 7 to 10 years.

Other actions for the promotion of innovation and technology transfer

Developing of equipment & scientific instrumentation devices carried out by the CeRTEV researchers:

• <u>E.B. Ferreira (EESC/USP)</u> and the team engaged in the research of glass sintering assisted by electrical field assembled the new furnace built in partnership with the WT Industry and the electrical field apparatus for flash sintering. The automatic optical dilatometry apparatus (Figure x) will be tested, and two M.Sc. graduate students started in 2019 new projects on Flash sintering of glasses under the supervision of E.B. Ferreira and collaboration of C. Magon (IFSC). Below there is a photo of the new furnace instrumented for flash sintering and optical dilatometry.

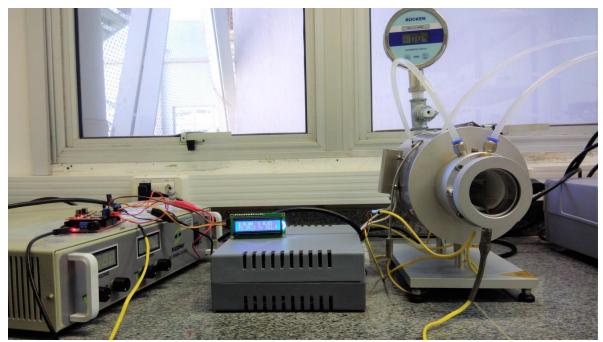


Figure x. New furnace instrumented for Flash sintering and optical dilatometry.

• M. Andreeta and O. Peitl (LaMaV/UFSCar) have ongoing activities on development and building an equipment for "Laser melting / aerodynamic levitation" with the possibility of applying electric fields in the melt (without electric current), detailed in the previous report. The continuity of this project depends on the approval of an equipment requested in the renewal of CEPID.

 <u>M. Nalin</u> is developing a solar mirror in partnership with Y. Messadeq, in a cooperation project between IQ-UNESP, Araraquara, and the University of Laval, Quebec/Canada. There is an interview on EPTV - Globo TV - about the subject scheduled shortly. The name of the project is "Energy concentrator coupled to optical fibers." Its function is to concentrate more efficiently the solar energy using mirrors coupled to an optical system (fiber optics) and to transport it to specific places. The system is flexible in responding to different purposes, for example, 1) disinfection of water by photocatalysis (original); 2) disinfection of animal manure; 3) drying of minerals; 4) lighting of large buildings; 5) heating water for the destruction of copper cyanide; (remediation); 6) machining of materials (3D manufacturing, cutting, etc.) (glass melting); 7) Desalination of seawater. The picture below (Figure xx) shows the prototype installed in the IQ-UNESP, Araraquara, SP.



Figure xx. A prototype of energy concentrator coupled to optical fibers installed in the IQ-UNESP, Araraquara, SP.

Other actions for the promotion of innovation and technology transfer

• <u>A.C.M. Rodrigues</u> supervised the M.Sc. project of Manoel da Cruz Barbosa Neto entitled "Development and characterization of low-cost vitreous-crystalline foam from industrial vitreous waste," namely, the automotive glass polishing waste supplied by the company **AGC**, Jundiaí, SP, for application as thermal insulation.

• <u>E.B. Ferreira</u> supervised the Final Paper of Nayme Salvatti Simões entitled "Algorithm for the calculation and maximization of packing density in ceramic mixtures."

• Lucas Pitaluga graduated as a materials engineer at UFSCar, had a project of Scientific Induction at LaMaV and participated in a project of Science Without Borders of CNPq in England. After graduating, he was contacted by the company **SCHOOT Float Glass** in Brazil by indication of professor <u>O. Peitl</u>, although the company has requested the appointment of an engineer with M.Sc. degree. Already at the beginning, the young engineer asked the LaMaV assistance in an industrial problem, which was resolved but not before generating a loss in the order of \$600,000 for the company. This is an emblematic case, which encourages other companies in the glass industry to hire materials engineers with training in CeRTEV.

• <u>A.C.M. Rodrigues</u> is part of the committee that organized the CeRTEV Course on Glass Technology 2019 for glass professionals, which will be held on August 19 to 24, with lecturers from the Glass Industry and University.

Glass-technology related articles

• Santos, G.G., Crovace, M.C., **Zanotto, E.D.**, *New engineered stones: Development and characterization of mineral-glass composites*, <u>Composites Part B:</u> <u>Engineering</u> 167 (2019) 556-565.

Elsayed, H., Rebesan, P., Crovace, M.C., Zanotto, E.D, (...), Colombo,
 P., Bernardo, E., *Biosilicate® scaffolds produced by 3D-printing and direct foaming using preceramic polymers*, Journal of the American Ceramic Society 102(3) (2019) 1010-1020.

• **Peitl, O., Zanotto, E.D**. - Bubbles-a glass-ceramic plague, Am. Ceramic Soc. Bulletin 2019, 98 (4), 30-33

• Fernandes, K.R., Parisi, J.R., Magri, A.M.P. **Zanotto, E.D.**, (...), Granito, R.N., Renno, A.C.M., *Influence of the incorporation of marine spongin into a Biosilicate®: an in vitro study*, 2019 Journal of Materials Science. Materials in medicine 30(6), pp. 64.

Baino, F., Verné, E., Zanotto, E.D., Fiume, E., (...), Brandão, S.M.,
 Schellini, S.A., *Bioactive glass and glass-ceramic orbital implants*, International Journal of Applied Ceramic Technology (2019).

o de Castro, T., Fares, H., Khalil, A.A., (...), Cardinal, T., Canioni, L., Nalin, M., *Femtosecond laser micro-patterning of optical properties and functionalities in novel photosensitive silver-containing fluorophosphate glasses*, Journal of Non-Crystalline Solids 517 (2019) 51-56.

Moraes, S.N.S., Morgado, D.L., Nalin, M., Application of Raman spectroscopy to industrial research: Determination of impurities in glass bottles, Vibrational Spectroscopy 100 (2019) 57-63.

Plan for the next period

• The CeRTEV Course on Glass Technology 2019 for glass professionals will be held on August 19 to 24, with lecturers from the Glass Industry and University.

• The CeRTEV Innovation and Technology-Transfer Coordination will organize and held the *3rd Workshop University-Industry on Glass Materials* at EESC-USP in São Carlos on October 31, 2019, aiming to probe demands on glass science and technology from the national glass industry.

• We will make an effort to boost the **Wikividros**, the Web-based content on glass science & technology, created by CeRTEV as an open collaboration platform hosted at https://wikividros.eesc.usp.br/.

• We will negotiate with partners the launching of a program of internship training and vacation school of undergrad and graduate students from CeRTEV in the glass industry, following the suggestion of Himanshu Jain, member of CeRTEV's IAB.

CeRTEV in the Media

• <u>https://engineering.unt.edu/news/du-study-advanced-glass-materials-</u> <u>fulbright-scholarship</u>

• <u>https://www.glass-international.com/news/view/three-postdoctoral-</u>

positions-open-at-certev-in-brazil

• <u>https://box.ufscar.br/48-curso-certev-de-tecnologia-vidreira-</u>

• <u>https://namidia.fapesp.br/novo-modelo-torna-mais-facil-prever-a-</u> cristalizacao-de-particulas-vitreas/188329

- <u>https://ceramics.org/award-winners/edgar-d-zanotto</u>
- <u>https://www.alfred.edu/about/news/pressreleases/viewrelease.cfm?ID=21</u> 098
- <u>https://www.pourlascience.fr/sd/physique/les-verres-coulent-ils-</u> 5995.php

• <u>https://www.suino.com.br/japao-quer-mais-parcerias-com-o-brasil-em-</u> <u>ciencia-e-tecnologia/</u>

• <u>https://www.funglass.eu/news/</u>

• <u>https://ceramics.org/ceramic-tech-today/biomaterials/additive-</u> manufacturing-offers-fast-and-simple-way-to-fabricate-bioactive-glass-ceramics

• <u>http://agencia.fapesp.br/material-bioativo-e-produzido-por-impressao-</u>

<u>3d/30799/</u>

Contracts - Official collaboration (signed contracts) with International Institutions

- Zanotto CeRTEV with FunGlass Institute, European Union
- Rodrigues, Zanotto, Peitl, Andreeta Clausthal University, Germany
- Rodrigues, Zanotto, Peitl, Andreeta Alfred University, USA in negotiation
- Rodrigues, Zanotto, Institut de Physique du Globe de Paris, France

- Rodrigues, Council of Scientific & Industrial Research (CSIR) and Central Glass & Ceramic Research Institute (CSIR-CGCRI), India

- Eckert, Westfälische Wilhelms Universität Münster, Germany

- Eckert, Shanghai Institute of Optics and Fine Mechanics (SIOM), China

- Eckert, University Rennes, University Montpellier, TU Munich, LMU Munich, University of Torino, University of Poznan, (EU-MaMaSELF)

- Nalin, Instituto de Química- DQGI-UNESP - Universidade de Bordeaux, França- FUNGlass H2020-MSCA-RISE-2018

-Nalin, Instituto de Química- DQGI-UNESP - Universidade de Laval - Quebec Canadá - JIRU (Joint International Research Unit)

Current Research Students and Post-docs working on glasses and vitreous materials 2019 - 2020

Current internship (IC) students working on vitreous materials			
Supervisão Edgar Dutra Zanotto			
Rodrigo C. Passos	IC	2017-2019	FAPESP
José Herculis Dantas de Araújo	IC	2018-2019	PIBIT- CNPq
Mayara Cerruti	IC	2018-2019	Serrapilheira
Nicoli Lucci	IC	2018-2019	FAPESP
Fernanda C. Puosso	IC	2018-2019	PIBIC - CNPq
Enzo Miguel	IC	2019 - 2020	FAPESP submetido
Supervisão Ana Candida Martins Rodrigues			
Lucas de Almeida Silva	IC	2018-2019	FAPESP
Supervisão Eduardo Bellini Ferreira			
Luís Gustavo Camargo Martos	IC	2017-2018	FAPESP submetido
Pedro Henrique Cardoso Mendes	IC	2019-2020	Sem bolsa
Levy Moreira Cruz	IC	2019-2020	Sem bolsa
Letícia Cursini	IC	2019-2020	Solicitará cota FAPESP do CeRTEV

		2017-2019	PUB-USP
André Balogh de Carvalho	IC	2019-2020	Solicitando novo projeto PIBIC-USP
		2018-2019	PIBIC-USP
Supervisão Jos	é Fab	ián Schneider	
Lucas Ely Bins Tsunaki	IC	2018-2019	FAPESP
Marc	elo Na	alin	
Ana Carolina Silva Sampaio	IC	2018-2019	FAPESP
Nicole Gouveia Roque	IC	2018-2019	VUNESP
Victoria Luisa Mameli	IC	2019-2020	PIBIC
Amanda Rodrigues Rossi	IC	2019-2020	PIBIC
Marcello I	R. <i>B</i> . <i>A</i>	Indreeta	
Matheus Henrique Ambrósio Santiago	IC	2018-2019	PIBIC
Rodrigo Seiji Ohtsuka	IC	2018-2019	Sem bolsa
Yasmim Yukimi Yamaguchi	IC	2018-2019	PIBIC
Marcelo Watanabe Machado	IC	2019-2020	Sem bolsa
Valmor R. Mastelaro			
Adrielle D Ricarte	IC	2018-2019	PIBIC

Current MSc and PhD stu	dents wo	orking on vitreou	s materials
Supervisão	Edgar L	Outra Zanotto	
Caroline Vidal	MSc	2018 - 2020	Sem bolsa
Geovana Lira	MSc	2018-2020	CNPq
Graziela Pentean Bessa	MSc	2017-2019	Ibar Refratários
Jeanini Jiusti	PhD	2016-2020	CNPq
Laís Dantas	PhD	2016-2019	CAPES
Claudia Abadia (Colombia)	PhD	2016-2019	CAPES
Maria H. Acosta (Colombia)	PhD	2017-2020	CNPq
Débora Mendes	PhD	2017-2020	CAPES

Bruna Valerini (w/Unesp)	PhD	2019-2021	solicitada
Lorena Rodrigues	PhD	2018-2021	CNPq
Supervisã	o Andrea	a Camargo	
Thiago Augusto Lodi	PhD	2018 - 2022	CNPq Institucional
Walter Faria Justi	PhD	2019 - 2023	CNPq Institucional
Marylyn Setsuko Arai	PhD	2019-2023	CNPq Insitucional
Iago Carvalho	MSc	2018 - 2020	CNPq Institucional
Supervisão Ec	luardo E	Bellini Ferreira	
Guilherme Silva Macena	PhD	2019 - 2023	CAPES Institucional
Johnata Cavalcanti Fonseca	PhD	2019 - 2023	CAPES Institucional
Karem Janeth Rimachi Hidalgo (Peru)	PhD	2018-2022	CAPES Institucional (coorientação Odonto Araraquara- UNESP)
Lucas Miguel Cândido	PhD	2016-2020	CAPES Institucional (coorientação Odonto Araraquara- UNESP)
Katherine Santos Oliveira	MSc	2019 - 2021	CAPES Institucional
João Matheus Rugeri Murdiga	MSc	2019-2021	CAPES Institucional
Supervisão M	arcello .	R. B. Andreeta	
Beatriz Gonçalves	MSc	2019 - 2021	CAPES
Supervisão And	a Cândic	la M. Rodrigues	
Adriana M. Nieto Muñoz (Colombia)	PhD	2016-2020	CNPq
Jairo Felipe Ortiz Mosquera (Colombia)	PhD	2016-2020	CNPq

Juliana Simões C. Licurgo	PhD	2018-2022	CAPES			
Manoel da Cruz Barbosa Neto	MSc	2017-2019	CAPES			
Supervisão	Supervisão Paulo Sergio Pizani					
Rafaella Bartz Pena	PhD	2017 - 2021	FAPESP			
Supervisão J	osé Schi	neider				
Gabriel Felipe Morguetto	MSc	2018 - 2019				
Supervisão	Oscar I	Peitl				
Tathiane Ferroeni Passos (com Clóvis Buzzato)	MSc	2017 - 2019	CAPES			
Supervisão H	ellmut	Eckert				
Henrik Bradtmueller (Alemanha)	PhD	2016-2019	DFG			
Millena Logrado	PhD	2016-2020	Nippon Electric Glass			
Supervisão Marcelo Nalin						
Leonardo V. Albino	PhD	2019-2022	CAPES			
Samira N. Stain	PhD	2019-2022	CAPES			
Juliana Moreno Paiva	PhD	2018-2021	CAPES			
Supervisão Valmor R. Mastelaro						
Vinicius Duarte Jesus	MSc	2019 - 2021	CAPES Institucional			

MSc and PhD students that graduated in 2017-2018-2019 / currently					
Supervisão Edgar Dutra Zanotto					
Gisele GuimarãesPhD2013 - 2017PD CNPq - LaMaV					
Renato Luiz Siqueira (co-Oscar Peitl)	PhD	2013 - 2017	Prof. private university		
André Hofmaister	MSc	2016 - 2018	Pilkington Glass		
Martha Velasco (Colombia)MSc2016 - 2017Univ. Colombia					
Supervisão Hellmut Eckert					

Carsten Doerenkamp	PhD	2013-2017	Postdoc, IFSC, USP
Lena Marie Funke	PhD	2015-2019	Postdoc, WWU Münster, Germany
Supervis	ão Mar	celo Nalin	
Antônio Eduardo de Souza	PhD	2015-2019	Coordenador Cursinho e Colégio Pandora
Roger Fernandes	PD	2019	Pós-doc - Alemanha
Supervisão Ana C	Candida	Martins Rodrig	ues
Rafael Bianchini Nuernberg	PhD	2014 - 2018	Pós-doutorado CEA – Marcoule- FR
Manoel da Cruz Barbosa Neto	MSc	2017-2019	Searching Job
Supervisão	Andrea	ı de Camargo	
Tassia Gonçalves	PhD	2014 - 2018	Faculty, Chemistry, UFMG Uberlandia
Marylyn Setsuko Arai	MSc	2016 - 2018	IFSC/USP
Patricia França Guidini	MSc	2016 -2018	Opto Eletrônica S/A, São Carlos
Walter José Gomes Juste Faria	MSc	2016-2019	IFSC/USP
Supervisão José	Pedro	Donoso Gonzale	27,
Igor d'Anciães Almeida Silva	PhD	2014 - 2018	Bolsista pós-doutorado FAPESP. Supervisor Prof.Hellmut Eckert
Eduar Enrique Carvajal Taborda (Colombia)	PhD	2014-2018	
Supervisão Eduardo Bellini Ferreira			
Raúl Julián Revelo Tobar (Colômbia)	PhD	2014-2018	Submitted a PIPE/FAPESP under analysis
Guilherme Silva Macena	MSc	2017-2019	Ph.D. at USP (CAPES)
Johnata Cavalcanti Fonseca	MSc	2017-2019	Ph.D. at USP (CAPES)
Supervisão Marcello R. B. Andreeta			
Ângela Santana Nunes	MSc	2017-2019	Bolsa CAPES

Current Post-Docs working on vitreous materials (grant good up to)					
Supervisão Edgar Dutra Zanotto					
Maziar Montazerian (Iran)	FAPESP	2020			
Azat Tipeev* (Russia) (w/Rino)	FAPESP	2021			
Gisele Guimarães	CNPq / AGC	May 2019 - August 2020			
Daniel Roberto Cassar	FAPESP	2021			
Alisson Mendes Rodrigues	CAPES	May 2019			
Mariana Villas Boas	Sem bolsa	2019			
Marina T. Souza	Vetra	2019			
Leila Separdar (Iran - w/ Rino)	FAPESP	August 2019 - 2022			
Supervisão Cláudio José Magon					
Carsten Doerenkamp (Alemanha)	PD	2019			
Supervis	são Hellmut Eckert				
Maria Costa (w/Ferreira)	FAPESP	2019			
Bianca Cerrutti	CNPq	2019			
Igor Danciaes	FAPESP	2020			
Lena Funke	DFG	2019			
Submitted	Cota FAPESP	2019			
Supervisão	Andrea de Camargo				
Gustavo Galleani	FAPESP	2019			
Leandro Piaggi Ravaro	CNPq	2019			
Kassio Papi Zanoni	FAPESP	2019			
Geysa Negreiros	FAPESP	2019-Recurso FAPESP			
Supervisão José Pedro Rino					
Azat Tipeev* (Russia) (w/ Zanotto)	FAPESP	2020			
Ary Rodrigues Ferreira Junior	PD	2019			
David Sampaio* (w/Pizani)	FAPESP	2019			
Leila Separdar (Iran) (w/Zanotto)	FAPESP	August 2019 - 2022			

Supervisão Ana Candida Martins Rodrigues				
Nilanjana Shasmal (Índia)	FAPESP	2020		
Karina Omuro Lupetti	FAPESP/Jornalismo	2019-2020		
Jéssica Fabiana Mariano dos Santos	FAPESP	Submetido		
Supervisão	Paulo Sérgio Pizani			
Benjamin Moulton (Canadá)	FAPESP	November 2019		
David Sampaio* (w/ Rino)	FAPESP	May 2019		
Thiago Rodrigues da Cunha	FAPESP	Cota FAPESP		
Supervisão Marcelo Nalin				
Douglas Faza Franco	FAPESP	2020		
Hssen Fares	FAPESP	2019		
Lia Mara Marcondes	CNPQ	2020		
Supervisão Eduardo Bellini Ferreira				
Maria Costa (w/ Eckert)	FAPESP	2019		
Supervisão Marcello R. B. Andreeta				
Rafael Bonacin de Oliveira	Sem bolsa	2019-2020		

GENERAL INFORMATION

Articles in scientific journals

Publications on vitreous materials (as of May 30, 2019)

 $\underline{https://scholar.google.com.br/citations?hl=pt-BR\&user=jqh7j5sAAAAJ}$

Highlighted articles in 2018 and 2019

*invited by editors, highly cited, most downloaded, awarded prizes, attracted

media attention, etc.

CASSAR, D.R., DE CARVALHO, A.C.P.L.F., ZANOTTO, E.D.; Predicting glass transition temperatures using neural networks, *Acta Materialia*, 159, pp. 249-256 (2018) - DOI: 10.1016/j.actamat.2018.08.022

https://ceramics.org/ceramic-tech-today/modeling-simulation/neural-networkspredict-glass-transition-temperatures

MASTELARO, V.R., ZANOTTO, E.D.; X-ray Absorption Fine Structure (XAFS) studies of oxide glasses-A 45-year overview, *Materials*, 11 (2), art. n° 204 (2018)

DOI: 10.3390/ma11020204 - ACCESS TYPE: Open Access (INVITED)

ECKERT, H.; Structural characterization of bioactive glasses by solid state NMR, *Journal of Sol-Gel Science and Technology*, 88 (2), pp. 263-295 (2018) – DOI: 10.1007/s10971-018-4795-7 (INVITED)

ECKERT, H.; Spying with spins on messy materials: 60 Years of glass structure elucidation by NMR spectroscopy, *International Journal of Applied Glass Science*, 9 (2), pp. 167-187(2018) - DOI: 10.1111/ijag.12333 (INVITED)

MOENKE, D. and ECKERT, H.; **Review on the structural analysis of fluoridephosphate and fluoro-phosphate glasses-** *JNCS X*, Frontiers issue, (2019) (**Invited review article**)

REIS, R. M.C.V. and ZANOTTO, E.D.; Simple model for particle transformation kinetics - Acta Materialia 2018, Spriggs Award for the best paper on phase equilibria in 2018 - awarded by the American Ceramic Society, May 2019.

ZANOTTO, E.D. and MAURO J.C.; **The glassy state of matter** - JNCS 2017, ELSEVIER, **Most downloaded paper of JNCS in 2017, 2nd in 2018** (26,000 papers available for downloading). Certificate given in **June 2019**, Boston. 4th most cited article in 2018.

MAURO, J.C., ZANOTTO, E.D.; - Two Centuries of Glass Research: Historical Trends, Current Status, and Grand Challenges for the Future -International Journal of Applied Glass Science (2014), 313-327 (amongst the 15 most cited articles of this journal ever)

DEUBENER, J., ZANOTTO, E.D. et al.; "Updated definition of glassceramics" - JNCS 2018, ELSEVIER, Most downloaded paper of JNCS in 2018. Certificate given in June 2019, Boston.

CROVACCE M.C., SOUSA M.T., CHINAGLIA C.R., PEITL O., ZANOTTO E.D., Biosilicate® - A multipurpose, highly bioactive glass-ceramic. In vitro, in vivo and clinical trials. JNCS 2016 - 10th most downloaded JNCS paper in 2018. Statistics of 2019

ELSAYED,H., REBESAN,P., CROVACE,M.C., ZANOTTO, E.D., COLOMBO, P., Enrico Bernardo - **Biosilicate® scaffolds produced by 3D-printing and direct foaming using preceramic polymers**, First published: 19 July 2018| <u>https://doi.org/10.1111/jace.15948</u>] Editor's choice in 2019

<u>https://ceramics.org/ceramic-tech-today/biomaterials/additive-manufacturing-</u> <u>offers-fast-and-simple-way-to-fabricate-bioactive-glass-ceramics</u>

VARSHNEYA, A.K., ZANOTTO, E.D., MAURO, J.C., Perspectives on the scientific career and impact of Prabhat K. Gupta Open Access, (2019) *Journal of Non-Crystalline Solids*: X 1,100011. (INVITED)

Papers on structure, dynamics, and properties of <u>vitreous materials</u> published in 2019 – <u>yellow = international collaborators</u>

(Source Scopus, June 18, 2019)

FERNANDES, R.G., REIS, R.M.C.V., TOBAR, R.R., ZANOTTO, E.D., FERREIRA, E.B., Simulation and experimental study of the particle size distribution and pore effect on the crystallization of glass powders, *Acta Materialia*, 175 (2019) 130-139, ISSN 1359-6454, https://doi.org/10.1016/j.actamat.2019.05.049.

ORTIZ-MOSQUERA, J.F., NIETO-MUÑOZ, A.M., Rodrigues, A.C.M., Precursor glass stability, microstructure and ionic conductivity of glass-ceramics from the Na 1+x Al x Ge 2–x (PO4)3 NASICON series, *Journal of Non-Crystalline Solids* 513 (2019) 36-43. **RODRIGUES, A.C.M.**, MUNHOZ, J.F.V.L., SANTAGNELI, S.H., DE OLIVEIRA, M., ECKERT, H., NALIN, M., Glasses in the NaPO3-WO3-NaF ternary system: preparation, physical properties and structural studies, (2019) *Journal of Non-Crystalline Solids* 505, pp. 379-389.

MARCONDES, L.M., RODRIGUES, L., RAMOS DA CUNHA, C., GONÇALVES, R.R., **DE CAMARGO, A.S.S.**, CASSANJES, F.C., POIRIER, G.Y., **Rare-earth ion doped niobium germanate glasses and glass-ceramics for optical device applications**, (2019) *Journal of Luminescence* 213, pp. 224-234.

RAJESH, D., DE CAMARGO, A.S.S., Nd3+ doped new oxyfluoro tellurite glasses and glass ceramics containing NaYF4 nanocrystals – 1.06 μm emission analysis, (2019) *Journal of Luminescence* 207, pp. 469-476.

LODI, T.A., DANTAS, N.F., GONÇALVES, T.S., **DE CAMARGO, A.S.S.**, PEDROCHI, F., STEIMACHER, A., **Dy3+ doped calcium boroaluminate glasses and blue led for smart white light generation**, (2019) *Journal of Luminescence*, 207, pp. 378-385.

SENTANIN, F., SABADINI, R.C., BARROS, S.C., SILVA, M.M., PAWLICKA, A., MAGON, C.J., Study of ionically conducting nanocomposites for reflective electrochromic devices, (2019) *Electrochimica Acta* 301, pp. 174-182.

SCHMELZER, J.W.P., ABYZOV, A.S., FERREIRA, E.B., FOKIN, V.M., Curvature dependence of the surface tension and crystal nucleation in liquids, (2019) International Journal of Applied Glass Science 10(1), pp. 57-68.

PEITL, O., ZANOTTO, E.D. - **Bubbles-a glass-ceramic plague**, *Am. Ceramic Soc. Bulletin* (2019), 98 (4), 30-33

SANTOS, G.G., CROVACE, M.C., **ZANOTTO, E.D.**, New engineered stones: **Development and characterization of mineral-glass composites**, (2019) *Composites Part B: Engineering* 167, pp. 556-565. FERNANDES, K.R., PARISI, J.R., MAGRI, A.M.P. **ZANOTTO, E.D**, GRANITO, R.N., RENNO, A.C.M., **Influence of the incorporation of marine spongin into a Biosilicate®: an in vitro study**, (2019) *Journal of materials science. Materials in medicine* 30(6), pp. 64.

SIQUEIRA, R.L., ALVES, P.F.S., DA SILVA MORAES, T., MARTINS, C.H.G., **ZANOTTO, E.D., Cation-doped bioactive ceramics: In vitro bioactivity and effect against bacteria of the oral cavity**, (2019), *Ceramics International* 45(7), pp. 9231-9244.

PRADO, S.C.C., **RINO, J.P., ZANOTTO, E.D.**, **Successful test of the classical nucleation theory by molecular dynamic simulations of BaS**, (2019) *Computational Materials Science* 161, pp. 99-106.

NUERNBERG, R.B., BELLO, T.S., FOKIN, V.M., ZANOTTO, E.D., RODRIGUES, A.C.M., Non-stoichiometric crystallization of Li2SiO3-CaSiO 3 glasses: Residual glass composition from ionic conductivity, 2019) *Journal of Non-Crystalline Solids* 510, pp. 158-165.

VARSHNEYA, A.K., ZANOTTO, E.D., MAURO, J.C., Perspectives on the scientific career and impact of Prabhat K. Gupta Open Access, (2019) *Journal of Non-Crystalline Solids*: X 1,100011. (invited paper)

ELSAYED, H., REBESAN, P., CROVACE, M.C., ZANOTTO, E.D, COLOMBO, P., BERNARDO, E., Biosilicate® scaffolds produced by 3D-printing and direct foaming using preceramic polymers, (2019) *Journal of the American Ceramic Society 102(3), pp. 1010-1020.*

BRADTMÜLLER, H., CERRUTTI, B.M., SOUZA, M.T., ZANOTTO, E.D., ECKERT, H., Structural characterization of boron-containing glassy and semicrystalline Biosilicate® by multinuclear NMR, (2019) *Journal of Non-Crystalline Solids* 505, pp. 390-399. MASTELARO, V.R., BAYER, P.S., ZANOTTO, E.D., Crystallization mechanism and kinetics of a Fe-diopside (25CaO.25MgO.50SiO₂) glass–ceramic, *Journal Materials Science* (2019) 54: 9313–9320.

ZHENG, Q., ZHANG, Y., MONTAZERIAN, M., MAURO, J.C, ZANOTTO, E.D., YUE, Y., Understanding Glass through Differential Scanning Calorimetry, (2019) *Chemical Reviews*, vol.x, p.x-xx.

MOULTON, B.J.A., RODRIGUES, A.M., SAMPAIO, D.V., ZANOTTO, E.D., PIZANI, P.S., The origin of the unusual DSC peaks of supercooled barium disilicate liquid, 2019) *Cryst.Eng.Comm.* 21(17), pp. 2768-2778.

BAINO, F., VERNÉ, E., ZANOTTO, E.D, FIUME, E., BRANDÃO, S.M., SCHELLINI, S.A., Bioactive glass and glass-ceramic orbital implants, (2019) International Journal of Applied Ceramic Technology.

DAGUANO, J.K.M.B., MILESI, M.T.B., RODAS, A.C.D., HORTELLANI, M.A., **ZANOTTO, E.D.**, **In vitro biocompatibility of new bioactive lithia-silica glassceramics**, (2019) *Materials Science and Engineering C* 94, pp. 117-125.

BENNDORF, C., DE OLIVEIRA JUNIOR, M., BRADTMÜLLER, H., PÖTTGEN, R., ECKERT, H., Rare-earth solid-state NMR spectroscopy of intermetallic compounds: The case of the 175 Lu isotope, (2019) *Solid State Nuclear Magnetic Resonance* 101, pp. 63-67.

FUNKE, L.M., JANKA, O., PÖTTGEN, R., GLEBOV, L., HANSEN, M.R., ECKERT, H., Short- and Medium-Range Order in Photothermal Refractive Glass Revealed by Solid-State NMR Techniques, (2019) *Journal of Physical Chemistry C* 123(19), pp. 12411-12422.

BRADTMÜLLER, H., UESBECK, T. ECKERT, H., MURATA, T., NAKANE, S., YAMAZAKI, H.; Structural Origins of Crack-Resistance on Magnesium Aluminoborosilicate Glasses Studied by Solid State NMR, (2019) J. Phys. Chem. C 123, 14941-14954. MUNHOZ, J.F.V.L., SANTAGNELI, S.H., DE OLIVEIRA, M., ECKERT, H., NALIN, M., Glasses in the NaPO3 -WO3 -NaF ternary system: preparation, physical properties and structural studies, (2019) *Journal of Non-Crystalline Solids* 505, pp. 379-389.

DE CASTRO, T., FARES, H., KHALIL, A.A., CARDINAL, T., CANIONI, L., NALIN, M., Femtosecond laser micro-patterning of optical properties and functionalities in novel photosensitive silver-containing fluorophosphate glasses, (2019) *Journal of Non-Crystalline Solids* 517, pp. 51-56.

GOMES FERNANDES, R., SQUINCA VALLE, P., FAZA FRANCO, D., NALIN, M., Crystallization kinetics study of silver-doped germanium glasses, (2019) *Thermochimica Acta* 673, pp. 40-52.

FRANCO, D.F., CARVAJAL, E.E., **DONOSO, J.P., MAGON, C.J., NALIN, M., Structural and EPR studies of Cu2+ ions in NaPO3 – Sb2O3 – CuO glasses**, (2019) *Journal of Non-Crystalline Solids* 503-504, pp. 169-175.

MORAES, S.N.S., MORGADO, D.L., NALIN, M., Application of Raman spectroscopy to industrial research: Determination of impurities in glass bottles, (2019) *Vibrational Spectroscopy* 100, pp. 57-63.

CASTRO, T., JUBERA, V., FARES, H., NALIN, M., RIBEIRO, S., Photoluminescence of Ag+ and Ag m n+ in co-doped Pr3+/Yb3+ fluorophosphate glasses: tuning visible emission and energy transfer to Pr3+/Yb3+ ions through excitation in different silver species, (2019) *Journal of Materials Science: Materials in Electronics.*

RODRIGUES, J.E.F.S., ROSA, W.S., FERRER, M.M., HERNANDES, A.C., GONÇALVES, R.V., **PIZANI, P.S., Spin-phonon coupling in uniaxial anisotropic** spin-glass based on Fe2TiO5 pseudobrookite, (2019) *Journal of Alloys and Compounds* 799, pp. 563-572.

BORGES, R., SCHNEIDER, J.F., MARCHI, J., Structural characterization

of bioactive glasses containing rare earth elements (Gd and/or Yb), (2019) Journal of Materials Science 54, pp 11390-11399.

DE OLIVEIRA, L.N., DO NASCIMENTO, E.O., ANDREETA, M.R.B., ANTONIO, P.L., CALDAS, L.V.E., Characterization of lithium diborate, sodium diborate and commercial soda-lime glass exposed to gamma radiation via linearity analyses, (2019) *Radiation Physics and Chemistry* 155, pp. 133-137.

Related works on scientometry, physics and chemistry of other types of materials

MONTAZERIAN, M., ZANOTTO, E.D., ECKERT, H., A new parameter for (normalized) evaluation of H-index: countries as a case study, (2019) *Scientometrics* 118(3), pp. 1065-1078.

SCIUTI, L.F., GONÇALVES, T.S., TOMAZIO, N.B., MENDONÇA, C.R., DE BONI, L., DE CAMARGO, A.S.S., **Random laser action in dye-doped xerogel with inhomogeneous TiO2 nanoparticles distribution**, (2019) *Journal of Materials Science: Materials in Electronics*.

ZANONI, K.P.S., VILELA, R.R.C., SILVA, I.D.A., MURAKAMI IHA, N. Y., ECKERT, H, DE CAMARGO, A. S. S., **Photophysical properties of Ir(III) Complexes Immobilized in MCM-41 via Templated Synthesis**, (2019) *Inorgan. Chem.* 58, pp. 4962-4971.

ECKERT, H., RADZIEOWSKI, M., STEGEMANN, F., DOERENKAMP, C., WITTSTOCK, G., JANKA, O., Correlations of Crystal and Electronic Structure via NMR and X-ray Photoelectron Spectroscopies in the RETMAl 2 (RE = Sc, Y, La-Nd, Sm, Gd-Tm, Lu; TM = Ni, Pd, Pt) Series, (2019) *Inorganic Chemistry* 58(10), pp. 7010-7025

ECKERT, H., JIE, X., DANILIUC, C.G., KNITSCH, R., KEHR, G., ERKER, G., Aggregation Behavior of a Six-Membered Cyclic Frustrated Phosphane/Borane Lewis Pair: Formation of a Supramolecular Cyclooctameric Macrocyclic Ring System, (2019) Angewandte Chemie - International Edition 58(3), pp. 882-886.

BENNDORF, C., DE OLIVEIRA, M., DOERENKAMP, C., ECKERT, H., PÖTTGEN, R., **11 B and 89 Y solid state MAS NMR spectroscopic investigations of the layered borides YTB 4 (T = Mo, W, Re)**, (2019) *Dalton Transactions* 48(3), pp. 1118-1128.

JANSEN, T., FUNKE, L.M., GOROBEZ, J., JÜSTEL, T., ECKERT, H., **Redemitting K 3 HF 2 WO 2 F 4 :Mn 4+ for application in warm-white phosphorconverted LEDs-optical properties and magnetic resonance characterization**, (2019) *Dalton Transactions* 48(16), pp. 5361-5371.

MICHELIN, J.V., GONÇALVES, L.G.V., RINO, J.P., On the transferability of interaction potentials for condensed phases of silicon, (2019) *Journal of Molecular Liquids* 285, pp. 488-499.

RIBEIRO-SILVA, C.I., PICININ, A., RINO, J.P., MENEZES, M.G., CAPAZ, R.B., **Temperature effects on the structural phase transitions of gallium phosphide**, (2019) *Computational Materials Science* 161, pp. 265-275.

CURCIO, A.L., MARTÍNEZ ESPINOSA, J.W., PIZANI, P.S., DE GIOVANNI RODRIGUES, A., Effects of cadmium insertion in blue-excited photoluminescence of ZnO, (2019) *Optical Materials* 89, pp. 344-348.

CUNHA, T.R., RODRIGUES, A.D., SAMPAIO, D.V., DA COSTA, R.C., PIZANI, P.S., Thermal expansion, compressibility and bulk modulus of ilmenitetype CoTiO3 : X-ray diffraction at high pressures and temperatures, (2019) *Solid State Sciences* 88, pp. 1-5.

LINO, A.V.P., COLMENARES CALDERON, Y.N., MASTELARO, V.R., ASSAF, E.M., ASSAF, J.M., Syngas for Fischer-Tropsch synthesis by methane trireforming using nickel supported on MgAl2O4 promoted with Zr, Ce and Ce-Zr, (2019) *Applied Surface Science* 481, pp. 747-760. ONOFRE, Y.J., CATTO, A.C., BERNARDINI, S., DA SILVA, L.F., DE GODOY, M.P.F., MASTELARO, V.R., **Highly selective ozone gas sensor based on nanocrystalline Zn0.95Co0.050 thin film obtained via spray pyrolysis technique**, (2019) *Applied Surface Science* 478, pp. 347-354.

RAKHSHA, A.H., ABDIZADEH, H., POURSHABAN, E., MASTELARO, V.R., MONTAZERIAN, M., Ag and Cu doped ZnO nanowires: A pH-Controlled synthesis via chemical bath deposition, (2019) *Materialia* 5,100212.

LAVINSCKY, A.B.S., WELSCH, A.-M., KENNEDY, B.J., BERNARDI, M.I.B., MASTELARO, V.R., Order-disorder phenomena and octahedral tilting in SrTi 1-XSnXO3 perovskites – A structural and spectroscopic study, (2019) *Journal* of Solid State Chemistry 269, pp. 521-531.

Books and book chapters published

DE CAMARGO, A.S.S., Glasses and glass-ceramics. A world without them? In Environments, technoscience and its relation to sustainability, ethics, aesthetics, health and the human future, Special Edition Brazilian Humboldt Kolleg, 179-187, Ed. Vania Gomes Zuin, Edufscar (2019)

ECKERT, H., Sol-gel synthesis of non-siliceous glasses and their structural characterization by solid state NMR, H. Handbook of Sol-Gel Science and Technology, Lisa Klein, ed. Vol. III, (2018), 1323-1373. (invited)

ZANOTTO, ED. and SMEDSKJAER, M. - *Frontiers of Glass Science, Special issue of JNCS X*, (2019), Organizers of the Frontiers of Glass Science Symposium, Foz do Iguaçu, Aug. 2018

The eight invited papers cover various aspects of the structure, dynamic processes, and properties of inorganic glasses. Advances in glass structure analysis are reviewed by Doris Möncke (Alfred University) and **Hellmut Eckert** (University of São Paulo) in "Review on the structural analysis of fluoride-phosphate and fluoro-phosphate

glasses", and several others.

Registered patents

M. NALIN and co-inventors filed the patent <u>17AUIN080</u> "*Product and process* for the preparation of oxide glasses and optical fibers for use in faraday rotators" (in Portuguese), March/2019, in the Brazilian National Institute of Industrial Property (INPI) as results of their scientific and technological efforts in a field of interest of our CEPID. The analysis at INPI, unfortunately, may take from 7 to 10 years.

Oral presentations at international and national conferences

INTERNATIONAL CONGRESSES, WORKSHOPS AND SYMPOSIA 2019

ZANOTTO, E.D. – "On the ultimate fate of glass" - 8th Otto-Schott Colloquium/ 4th Entropy workshop, Jena, Germany, Sept. 2019 (INVITED, committed)

ZANOTTO, E.D. – "On my fun and educational 3-decade interaction with the glass guru-

Arun Varshneya Festschrift", **ICG 2019 - 25th International Congress on Glass**, Boston, USA, June 2019 (INVITED)

CASSAR, D.R. and ZANOTTO, E.D. – "On the breakdown of the CNT" - ICG **2019** 25th International Congress on Glass, Boston, USA, June 2019 (INVITED)

NALIN, M. – "Heavy metal oxide glasses containing luminescent rare-earth single crystals", **ICG 2019 - 25th International Congress on Glass**, Boston, USA, June 2019 (ORAL)

SANTAGNELI S., ECKERT, H. NALIN, M., - "Using Solid State NMR and Raman Spectroscopies to solve short and long-range order in fluorophosphate glasses", **ICG 2019 - 25th International Congress on Glass**, Boston, USA, June 2019 (ORAL)

RODRIGUES, A.C.M, - "Inferring the chemical composition of the residual glassy phase of glass-ceramics from ionic conductivity", **ICG 2019 - 25th International Congress on Glass**, Boston, USA, June 2019 (ORAL)

RODRIGUES, A.C.M, "First Glass Technician Training Course in South America", **25th International Congress on Glass**, Boston, USA, June 2019 (ORAL)

ECKERT, H., "Network former mixing (NFM) effects in phosphate glasses.

Structure/property correlations studied by modern solid-state NMR techniques", International Congress on Glass and GOMD, American Ceramic Society Meeting, June 2019 (INVITED)

ECKERT, H.,"Sol-Gel Synthesis of Non-Siliceous Glasses and Structural Characterization by Solid State NMR", **International Congress on Glass and GOMD**, American Ceramic Society Meeting, Boston June 2019 (**INVITED**).

MURATA, T., KATO, Y., NAKANE, S, ECKERT H., "Relationship between mechanical properties and network structure of the aluminoborosilicate glasses of 20 Na2O-x B2O3-(20-x)Al2O3-60SiO2", **International Congress on Glass and GOMD**, American Ceramic Society Meeting, Boston June 2019 (CONTRIBUTED TALK).

D ÀNCIAES ALMEIDA SILVA, RODRIGUEZ, A.C., ECKERT, H., NIETO-MUNOZ, "Structure/property correlations on new Li1.5M0.5Ge1.5(PO4)3 (M= Sc, Ga, Y) NASICON glass ceramics by impedance spectroscopy and solid-state NMR", **International Congress on Glass and GOMD**, American Ceramic Society Meeting, Boston June 2019 (CONTRIBUTED TALK).

C.DOERENKAMP, E. CARVAJALÇ, W. FARIA, J. DONOSO, A.S.S. DE CAMARGO, J. MAGON, H. ECKERT, "Composition-Structure-Property Correlations in Rare-Earth doped heavy metal oxyfluoride glasses", **International Congress on Glass and GOMD**, American Ceramic Society Meeting, Boston June 2019 (CONTRIBUTED TALK).

S.H. SANTAGNELI, G. GALLEANI, H. FARES, M. NALIN, H. ECKERT, "Using solid state NMR and Raman spectroscopies to solve short-and medium-range order in fluorophosphate glasses", **International Congress on Glass and GOMD**, American Ceramic Society Meeting, Boston June 2019 (CONTRIBUTED TALK).

G. GALLEANI, C. DOERENKAMP, S. SANTAGNELI, A. DE CAMARGO, H. ECKERT, "Structure-properties relations in rare-earth doped indium fluoride phosphate glasses studied by solid state NMR, EPR and optical spectroscopic strategy", **International Congress on Glass and GOMD**, American Ceramic Society Meeting, Boston June 2019 (CONTRIBUTED TALK).

J. REN, H. ECKERT, "Superstructural units involving six-coordinated silicon in sodium phjosphosilicate glasses studied by advanced NMR methodology", **International Congress on Glass and GOMD**, American Ceramic Society Meeting, Boston June 2019 (CONTRIBUTED TALK). N. STONE-WEISS, N. J. SMITH, R. YOUNGMAN, E.M. PIERCE, H. ECKERT, A. GOEL, "Understanding structure-degradation behavior relationships in Na₂O-P₂O₅-B₂O₃-SiO₂ based model bioactive glasses", **International Congress on Glass and GOMD**, American Ceramic Society Meeting, Boston June 2019 (CONTRIBUTED TALK).

MACENA, G.S., FOKIN, V., ABYZOV, A.S., ZANOTTO, E.D., FERREIRA, E.B., "Crystallization kinetics of non-stoichiometric Na₂O·2CaO·3SiO₂– Na₂O·3CaO·6SiO₂ glasses", **25th International Congress on Glass**, Boston, USA, June 2019 (ORAL)

UNUABONAH, E.I., DE CAMARGO, A.S.S., Water disinfection by low cost hybrid clay photocatalysts", 3rd World Forum for Women in Science without Borders, Cairo, Egypt, March 2019 (INVITED)

DE CAMARGO, A.S.S., "Efficient host-guest luminescente materials for photonic and biophotonic applications", Humboldt Kolleg "Breaking Paradigms towards a Multi-, Inter- and Transdisciplinary Science", **250th Birthday of Alexander von Humboldt**, Ibarra, Equador, February 2019 (INVITED)

NATIONAL MEETINGS 2019

RINO, J.P – "Molecular dynamics study of spontaneous nucleation and crystallization in barium sulfide", *THEORY and SIMULATION II, Encontro de Outono de Física, Sociedade Brasileira de Física*, 26-31/May, 2019, Aracajú, SE (ORAL)

ZANOTTO, E.D. – "Pesquisa em novos materiais vítreos no Estado de SP", Sao Paulo, March 31, *Japan-Fapesp technology symposium*, 2019 (INVITED)

MASTELARO, VR – "The XAFS technique Applied to the study of the atomic and electronic structure of inorganic materials" *WORKNANO 2019 – Materials science addressed with modern analytical and theoretical methods*. 21st – 22nd February 2019, IFUSP, USP São Paulo. (INVITED)

ZANOTTO, E.D. – "Entendimento e desenvolvimento de materiais funcionais pelo LaMaV" - *CeRTEV, I SPIMF*, Sao Carlos, May 2018 (INVITED)

Invited seminars delivered at universities and companies

DE CAMARGO, A.S.S., Física para Meninos e Meninas, Escola Física Contemporânea IFSC/USP, São Carlos, July 2019 (committed)

NALIN, M - GLASSGLASS Project - Université de Bordeaux - May 2019

DE CAMARGO, A.S.S., Universidade de Muenster, Seminário: Oportunidades de Pesquisa na Alemanha, **IFSC/USP**, São Carlos, May 2019

NALIN M. - GlassGlass Project - Magnetic Glasses - Instituto de Física -Universidade de São Paulo, São Paulo-SP, April 2019

ECKERT, H. New Magnetic Resonance Approaches for the Structural Characterization of Ion Conducting and Photonic Glasses, Department of Chemistry, **Universidade de Santiago de Chile**, March 2019.

ZANOTTO, E.D. - Glass-ceramics, past, present and future, AGC, Japan, January 2019

Conferences, workshops and symposia organized or co-organized by Certevians

ZANOTTO, E.D. and KELTON, K.F. - Fundamentals of glass crystallization-**Symposium during the ICG 2019**, Boston, USA, June 2019

DE CAMARGO, A.S.S., Oportunidades de Pesquisa na Alemanha, São Carlos – SP. Organizadora, **IFSC/USP**, May 2019

ECKERT. H. Workshop on Solid State NMR, International Masters Program MaMaSELF, University of Montpellier, February 2019

Awards and distinctions granted to CeRTEV faculty in the period January -June 2019

ACOSTA, M.H.R.; CASSAR, D.R.; ZANOTTO, E.D. - Unmasking the breakdown of the Classical Nucleation Theory - Awarded the **best poster** presented at the ICG 2019, Boston, June (competed with 140 posters)

ZANOTTO, E.D. & former student REIS, R.M.C.V. - Acta Materialia article 2018, **Spriggs Award** for the best paper on phase equilibria in 2018 - awarded by the

American Ceramic Society, May 2019.

ZANOTTO, E.D. - "S. Scholes Lecture Award" invitation by the Dean of Engineering - Alfred University, Alfred, NY, April 2019

DE CAMARGO, A.S.S., Nippon Foundation Overseas **Research Grant**, Japan, March 2019.

Short courses delivered

ECKERT, H, DE CAMARGO, A.S.S. Solid State Spectroscopy, University of Montevideo, Montevideo, Uruguay, November 2019 (COMMITTED)

DE CAMARGO, A.S.S., Angular momentum spectroscopy applied to characterization of sol gel materials, Buenos Aires, Argentina, October 2019. (COMMITTED)

ECKERT, H., Spectroscopy and the Structure of Matter, WWU Münster June/July 2019

MASTELARO, VR, Espectroscopia de Fotoelétrons Excitados por Raios-X (XPS): Fundamentos, Aplicações e Análise de dados, Universidade Estadual de Ponta Grossa, June 2019.

Editorship of scientific journals in 2019

ECKERT, H. - Editorial Board Member, Solid State Nuclear Magnetic Resonance (Elsevier)

ECKERT, H. - Editorial Board Member, Zeitschrift für Naturforschung, (Physics), de Gruyter

ANDREETA, M.R.B. - Associate Editor: Open Chemistry Journal (ISSN: 1874-8422)

ANDREETA, M.R.B. - Editorial Board Member, EUREKA: Physics and Engineering (ISSN 2461-4254 (Print))

MASTELARO, V. - Member of the Editorial Commission of Materials Research: Ibero-american Journal of Materials

MASTELARO, V. - Associate Editor: Journal of Alloys and Compounds (Elsevier)

RODRIGUES, A.C.M. - Associate Editor, Frontiers in Materials: Glass Science

ZANOTTO, E. D. - Editor of the Journal of Non-Crystalline Solids since 2010

ZANOTTO, E. D.- Member of the International Advisory Boards of: International Journal of Applied Glass Science (USA), Materials Research (Ibero-American), Bulletin de la Sociedad Espanhola de Ceramica y Vidrio (Spain), Biomedical Glasses (Germany), Iranian Journal of Materials Science and Engineering (Iran), Cerâmica (Brazil), Springer-Nature Applied Sciences (UK), International Materials Reviews (UK), Ceramics in Modern Technologies (Italy).

Administrative and consulting role in scientific societies in 2019

DE CAMARGO, A. S. S. - Membro do Conselho, Clube Humboldt do Brasil, desde 2014.

DE CAMARGO, A. S. S., Co-organizadora do 4th Forum of Women in Science without borders, a ser realizado em Rio de Janeiro - RJ em Fevereiro de 2020.

DE CAMARGO, A. S. S., Coordenadora da Área de Óptica no EOSBF - Encontro de Outono da Sociedade Brasileira de Física, a ser realizado em Bonito - MS em Maio de 2020.

DE CAMARGO, A.S.S. Membro (Diretora Científica) da chapa única apresentada à SBPMat para eleição da nova diretoria em Agosto de 2019.

RODRIGUES, A.C.M. - Chair of the ICG TC23: Education in Glass

NALIN, M. - Member of the ICG TC20: Optoelectronics

FERREIRA, E. B. – Glass Committee of the Brazilian Ceramic Society

ECKERT, H. - Advisory Board member, Network of the French High-Field NMR **Facilities**

ECKERT, H. - Hans - Hellmuth Vits-Prize Committee, Society of the WWU Münster

ECKERT, H. - Awards Committee, European Research Council

ECKERT, H. - Georg-Forster Prize Committee, Alexander-von-Humboldt Foundation

ECKERT, H. - Georg-Forster Fellowship Selection Committee, Alexander-von-

Humboldt Foundation

ECKERT, H. - Member, Board of Coordinators, Physics, FAPESP

ZANOTTO, E.D. - President of the Scientific Council of the Serrapilheira **Institute until April 2019**

ZANOTTO, E.D. - President of the Curators Council of the São Carlos TechParq

ZANOTTO, E.D. - Board of Directors of the Brazilian Ceramic Society

ZANOTTO, E.D. - Brazilian representative in the **International Commission on Glass**

ZANOTTO, E.D. - Council member of the International Ceramic Federation
ZANOTTO, E.D. - Council member of the FunGlass Institute, European Union
ZANOTTO, E.D. - Council Member of the Serrapilheira Institute
ZANOTTO, E.D. - Council Member of IMPA (Institute of Mathematics), Brazil
ZANOTTO, E.D. - Member of the Glass Crystallization / GC Committee: ICG

TC07

ZANOTTO, E.D. - Engineering Fellowship Selection Committee, TWAS
 ZANOTTO, E.D. - G.W. Morey Award Selection Committee, GOMD - ACerS
 ZANOTTO, E.D. - Gottardi Prize, Voting Committee, ICG
 ZANOTTO, E.D. - Zachariasen and Mott Awards, Selection Committee, JNCS
 ZANOTTO, E.D. - Fellowship Selection Committee, Young researchers SP
 session- Brazilian Academy of Sciences

ZANOTTO, E.D- CBMM Prize Selection Committee, CBMM

ZANOTTO, E.D. - Sao Carlos Scientist of the Year Award committee, **Prefeitura** de São Carlos

International (short and long term) visitors in 2019

Dr. Alexander Abyzov – Ukraine Dr. Vladimir Fokin- St. Petersburg Prof. Jean-Louis Souquet- Grenoble Dr. Harold Lozano - Santiago, Chile Prof. Phil Salmon - Bath, UK

Voluntary activities within the respective universities

DE CAMARGO, A. S. S. - Vice-Presidente Comissão de Pesquisa IFSC - 05/16 - atual

DE CAMARGO, A. S. S. - Membro titular da Comissão de Pós Graduação Ciência e Engenharia de Materiais, EESC/USP - 08/14 - atual

DE CAMARGO, A. S. S. - Membro titular da Comissão Coordenadora do Curso

de Bacharelado em Química, IQSC/USP - 03/17 - atual

DE CAMARGO, A. S. S. - Membro titular do Conselho de Depto. Física e Ciência Interdisciplinar, IFSC/USP – Maio/16 - atual

DE CAMARGO, A. S. S. - Membro titular da Congregação do IFSC/USP, IFSC/USP – 08/16 - atual.

DE CAMARGO, A. S. S. - Membro da Comissão de Assessoramento da Chefia do Dept. de Física e Ciência Interdisciplinar para elaboração do plano institucional departamental (2018-2023)

ECKERT, H. - Membro titular de Comissão Relações Internacionais (CRINT)

ECKERT, H.- Membro titular do Conselho de Depto. Física e Ciência Interdisciplinar, IFSC/USP.

ECKERT, H. - Membro titular da congregação do Instituto de Física São Carlos (IFSC), USP.

NALIN, M – Membro da congregação do IQ-UNESP – Araraquara (2014-atual)

NALIN, M – Representante do IQ-UNESP no Conselho Universitário da UNESP-(11/2016-2018)

NALIN, M - Chefe do Departamento de Química Geral e Inorgânica, IQ -UNESP, Araraquara - (2017-2020)

FERREIRA, E.B. - Membro Titular do Conselho do Departamento de Engenharia de Materiais, EESC/USP, 2018 – atual.

FERREIRA, E. B. - Suplente da Comissão de Pesquisa, EESC/USP, 2017 - Atual

FERREIRA, E. B. – Membro suplente da Comissão Coordenadora do Curso de Engenharia de Materiais, EESC/USP, 2018 – atual.

ZANOTTO, E.D. - Member of the Research Council (CoP) of UFSCar since 2013.

ZANOTTO, E.D. - Vice-chair of the ceramics area of DEMa / UFSCar since 2016. ZANOTTO, E.D. - Supervisor of the LaMaV / UFSCar since 1977.

ANDREETA, M. R. B. - Coordenador da atividade de extensão: ACIEPE -"Engenheiros e Cientistas do Futuro" oferecida semestralmente (4 créditos).

ANDREETA, M. R. B. - Vice-coordenador da área de Materiais Cerâmicos-

DEMa - UFSCar (6/2019 - 6/2021)

ANDREETA, M. R. B. - Membro suplente da Coordenadoria de Iniciação Científica e Tecnológica (CCET Tecnológicas - Campus São Carlos) - 2018/2020.

SCHNEIDER, J.F. – Coordenador do Curso de Bacharelado em Física, Instituto de Física de São Carlos/USP, 2016 – atual.

SCHNEIDER, J.F. – Membro da Comissão de Graduação, Instituto de Física de São Carlos/USP, 2016 – atual.

RINO, J.P. – Membro titular representante do CCET para avaliação e desempenho acadêmico dos docentes.

MASTELARO VR- Membro Titular junto ao Conselho Departamental FCM desde 04.02.2010.

MASTELARO VR- Vice-chefe do Departamento de Física e Ciências dos Materiais desde 05/2016

MASTELARO VR- Membro Titular junto a congregação do IFSC desde 05/.2018.

DONOSO, G.J. - Membro da Comissão de Cultura e Extensão, IFSC - USP (desde 2018)

Funding from industry 2019 - 2020

E.D. ZANOTTO

-ACG (Japan)	Euros 76,200 Aug. 2019-2020
-IVOCLAR AG	Euros 54,000 Set.2019 – Aug.2020

HELLMUT ECKERT

-Nippon Glass	Euros 40,000 one year
- Schott Glass	Euros 30,000 in negotiation

MARCELLO R. B. ANDREETA

-Alacer Biomédica (R\$ 79.400, 00) jan.2019 - nov. 2019 -ENGECER (in negotiation - PIPE)

ANA CANDIDA MARTINS RODRIGUES

-ICG - International Commission on Glass Euro 2.000

A.S.S. DE CAMARGO

-Nippon Sheet Glass Foundation, US\$ 3.000,00

Funding from other agencies: CNPq, CAPES, internacional

H. Eckert, CNPq, Universal - R\$ 37,500 2019-2021
H. Eckert, DFG, SFB858. - €156,750, 2019-2021
H. Eckert, DFG, Ec168-20 € 10,000, 2019-2021
E.D. Zanotto, CNPq, Universal - R\$ 40.000 2019-2020
A.S.S. de Camargo, CNPq, Universal - R\$ 84.000,00 2016-2019
V. R. Mastelaro, CNPq, Universal, R\$ 90.000,00 - 2018-2021
J. Pedro Donoso: Chamada de Propostas Colaborativas FAPESP - Conicyt - Chile., FAPESP: R\$ 77.400,00 Conicyt - Chile: US\$ 50.000 (submetido)

Prestigious CNPq fellowships/grants to the CeRTEV faculty

ECKERT, H., Bolsa CNPq, Nível 1A -ZANOTTO, E.D., Bolsa CNPq, Nível 1A PIZANI, P.S., Bolsa CNPq, Nível 1B RINO, J.P. Bolsa CNPq, Nível 1B MASTELARO, V.R., Bolsa CNPq, Nível 1B DE CAMARGO, A. S. S., Bolsa CNPq, Nível 1D SCHNEIDER, J., Bolsa CNPq Nível 2 DONOSO J.P., Bolsa CNPq Nível 2 NALIN, M., Bolsa CNPq Nível 2 RODRIGUES A.C.M. Bolsa CNPq, Nível 2

Overall budget of our Center from other sources 2019-2020

Funded Projects by CAPES and CNPq	R\$ 251.500,00
International funds including student fellowships	Euro 166.750,00
CNPq Fellowships to professors	R\$ 236.400,00
Student IC, MSc, Dr, PD / grants from other sources	R\$ 1.313.616,00
Grants from companies	Euro 174.200,00 / R\$ 79.400,00
Prof. salaries USP, UFSCar, UNESP	R\$ 3.178.000
Staff salaries UFSCar, USP	R\$ 600.000,00

Evaluation of the CeRTEV report 2017-18 (5th year) by the IAB members (final)

Dr. Shingo NAKANE

CERTEV has been developing outstanding research of glass and glass-ceramics for various applications, which are structural reinforcement, bioactive, ion conductors, photonic, and catalytically active materials. They have released many original research articles to leading journals in inorganic, physics, and chemistry, surprisingly almost 100 articles in 2017-2018. In addition of the articles, the research have been presented in many international conferences by the members as invited and keynote lecture, leading to activate glass science internationally (for example, Annual Meeting of ICG Yokohama in Japan 2018, 12h International Symposium on Crystallization in Glasses and Liquids Segovia 2017, and Glass and Optical Materials Division San Antonio 2018). From my industry point of view, fundamental research of glass structure and crystallization are impressive. Understanding of glass structure and crystallization in atomic or nano level is difficult by industry themselves because of shortage of good apparatus and technique with well-educated researcher. Other impressive point is that the fundamental researches have been done not only by experiment, but also computational science (Molecular Dynamics Methods, MD). As conjugation of computational science start to be extremely active in any science fields all over the world, I believe CERTEV will establish a new way of application of MD to strengthen the fundamental research with continued outstanding success in the project.

CERTEV also develops a way for access of glass science to much broader people beyond specialists, especially to young prominent students and scientists by steady efforts with strategy of organizing seminar, short course and events.

In conclusion, CERTEV is promoting research and education internationally, and they have contributed development of the glass and glass-ceramics science by creation of fundamental knowledge and methods in this period 2017-18.

Otsu Shiga JAPAN, June 17th, 2019 Dr. Shingo Nakane, Division Manager in Nippon Electric Glass Co; Ltd. Fundamental Technology Division Phone: 81 (0)77 537 1381, <u>snakane@neg.co.j</u>

July 20th, 2019,

Kei Maeda, Fellow, AGC Inc.

It is an outstanding performance that approximately 100 papers has been published by major world-famous journals in glass science and technology during in this short period. That is an evidence that CeRTEV is continuing strong activities in the field of glass and glass-ceramics, and leading their progress for both scientific and technological aspects. As one of the typical examples, a new approach to investigate crystallization process by using in-situ Raman spectroscopy is worth noting. It successfully described the structural evolution of crystalline phase from supercooled barium disilicate melt. It is expected that further understanding on crystallization kinetics can be made combining with other techniques including transmission electron microscope (TEM), X-ray absorption fine structure (XAFS), etc. A molecular dynamic simulation is also a strong tool to understand the structure of glass. However, its application to crystallization kinetics of oxide glass is still problematic because of the limited time order of the simulation. A breakthrough is also expected.

Another important note is that CeRTEV provided some review articles including XAFS and nuclear magnetic resonance (NMR) techniques in this period. A review of

XAFS studies on oxide glass is written based on more than 160 references and summarizes 45 years history of this technique. The principle and appropriate examples are well described in the article, so that readers, even unfamiliar with this technique, can easily understand. It is a very good handbook for young researchers, who begin to use this technique.

Finally, there is a fact that the article entitled "Updated definition of glassceramics" published in Journal of Non-crystalline Solids (JNCS) was awarded by Elsevier as the most downloaded JNCS article in 2018, evidencing people pay a great attention to glass-ceramic materials. CeRTEV definitely plays an important role in this field. Further contribution of CeRTEV is expected to realize a big impact on glass industry.

Assessment of CeRTEV Performance Period: 2017-2018

Josef W. Zwanziger, CeRTEV IAB Member

Dept. Of Chemistry, Dalhousie University, Halifax, NS Canada 21 June 2019

My assessment is based on the document REPORT 5 2017-2018, supplied by Dr. Zanotto, and on the IAB meetings with Dr. Zanotto and other CeRTEV members, most recently in Boston, June 2019. I find in general that the CeRTEV lab continues to perform excellently in all aspects, including basic research; training of highly-qualified personnel; community outreach; and technology transfer. It is clear from the report that on the technical side, the focus emphasizes a longer-term strategy of fundamental science and development, rather than a short-term focus of bringing products to the market-place. I think that is a very appropriate target for a university-based research centre. Glass being an exceptionally practical material, of course it is appropriate that many of the research targets are glass and ceramic systems of relevance to application. To this end I am particularly impressed with the recent work on high-strength glass-ceramics, and bioactive glasses. These two areas have many possibilities both for fundamental advances and for valuable products. The ion conducting glass work, on the other hand, I would suggest should be somewhat refocused away from glass compositions that are rich in chemically interesting but very impractical species such as Cr, Ge, and Sr, and focused more on systems that are cheaper and more environmentally benign.

The various training programs that the centre has developed appear excellent and useful, and the group is clearly fully invested in outreach. Very often these days "outreach" is obviously an afterthought not taken seriously, but not so with CeRTEV, and programs here are innovative and interesting.

Broadly, this centre is without question fulfilling its mission, and is viewed internationally as on of the key glass research centres in the world.

Himanshu Jain

Lehigh University, USA

I would like to congratulate the CerTEV team of investigators including faculty members, research scholars and graduate students for keeping the momentum of high productivity of research on the main topics of glass science and engineering that were proposed in the original proposal. It is often quite difficult to maintain a balance of fundamental scientific advancements that may benefit the society in the long run and engineering innovations that could impact in the short run. The challenge of converting new ideas into invention, invention into innovation, innovation into products, products into benefit to society is a long process. The success of this highly entangled process depends on so many factors that re well beyond the capabilities of researchers. Nevertheless, CerTEV has been striving hard and keeps advancing the process forward, and I think it is making significant progress in this direction. I especially appreciate the attempt of its leaders to reach out to international companies that may be in a stronger position to make use of the expertise and know how developed by CerTEV researchers.

The standard output of researchers is publications. For CerTEV it remains at the top among world's academic institutions involved in glass research. This is remarkable and testimony to the sustained hard work of CerTEV scientists. I especially like the significant fraction of publications as review/invited articles in leading materials science journals. It helps other researchers, especially who are in neighboring fields, to learn the subject matter, and also enhances the recognition of the authors and their institutions. Great job!

I would like to make one suggestions for the future: try to establish internship and summer research opportunities for the students to work in industry. It gives the students a valuable exposure to the real life and helps them see the value of what they are learning in school. It also helps the faculty build professional relationship with colleagues in companies, which may lead to research collaborations, consulting projects, etc. It can be a win-win program if managed carefully.

Himanshu Jain

Mark J. Davis, Ph.D

The mission, scope, and activities of CerTEV continue to put this organization at the forefront, internationally, of glass-related research. The breadth of its activities is matched by the diverse talents that CerTEV brings to bear on the various problems the center focuses on. As one example, recent work by José Pedro Rino, a physicist with deep experience in computational modeling, in conjunction with colleagues from the more traditional glass and glass-ceramic related disciplines, has already made new and impactful insights into to what extent classical nucleation theory actually constitutes a useful theory, a long-standing unresolved issue. It was precisely the combination of diverse backgrounds that, I believe, led to this significant new contribution. I look forward to more such interactions between fields that don't necessarily "speak" to one another and I wish the center continued success.

Mark J. Davis, Ph.D. Senior Principal Scientist Research and Technology Development SCHOTT North America, Inc.

Yuanzheng Yue

Assessments on CeRTEV in 2017-2018

In the past two years, CeRTEV has achieved substantial advances in glass science and technology, particularly, concerning fundamental glass problems, crystallization, bioactive glass and glass-ceramics, functional glasses, glass and glass-ceramics for energy applications. These advances have been presented in the glass community and beyond, and reflected in numerous high-impact scientific papers, conference talks (especially invited ones), and patents. Besides the outstanding management of center leaders and principal investigators, and the enthusiastic creative engagement of their team workers, the success of CeRTEV is also strongly associated with its strong international collaboration network. Today the center has become an open dynamic forum that have been attracting both senior and young scientists from around world. As a member of the International Advisory Committee of CeRTEV, In the last two years I had a tight collaboration with Professor Zanotto and his postdoc Maziar Montazerian, which led to a highly influential review article "Understanding glass by DSC" published in Chemical Reviews (Impact factor: 54).

CeRTEV has made great progress in transforming their scientific findings and results into industrial technology and innovation. This was done by taking the visionary strategy: establishing cooperation agreements with industry; attempting to build spin-off companies; and promoting technology transfer.

CeRTEV has made great contributions to education of young researchers by organizing the Meetings of the Technical Committee (TC) for Education (under ICG), conferences, workshops, PhD courses, and other events. They put high values on connections between glass science, technology and education. The TC for Education, which is led by Professor Ana Cândida Martins Rodrigues is one of the most active TCs in ICG.

Based on the outstanding research environments established in the past 5 years, CeRTEV has a huge potential to be further developed and to deliver highly original results to scientific communities and society. I wish the center to invest more effort in fundamental and interdisciplinary research, and publish even more high-impact papers in future. I am confident that CeRTEV will continue to be a successful leading research center in the world.

Yuanzheng Yue, Professor, PhD yy@bio.aau.dk Aalborg, June 23, 2019

Prof. Joachim Deubener

Report on activity of CeRTEV in the period Dec 2017 – Dec 2018

My assessment on the main activities of CeRTEV with respect to fundamental research, education & outreach and technology transfer is based on the information provided during the annual board meeting, discussion with the PIs at the International Congress on Glass in Boston, June 9-14, 2019 and the delivered report No. 5.

Fundamental Research

Through this information, it becomes clear that the outstanding achievements of CeRTEV have definitely continued in 2018. The numbers of publications in prestigious peer-reviewed journals is extremely high. In the period, 64 papers have been published. These publications were prepared to a large share by participation of researchers from abroad, which emphasizes the improved international visibility and connectivity of CeRTEV in fundamental scientific research. In particular, papers of exceptional quality on glasses and glass-ceramics are covering the main topics of CeRTEVs research agenda, such as fundamental aspects and definitions of their formation and transformation, high-strength, bioactivity, ion conductivity for advanced batteries, sealing for fuel cells as well as photonic properties.

Education and Outreach

PIs of CeRTEV have received a high level of national and international recognition on scholar and educational issues. Memberships and appointments in boards, councils and technical committees of international organizations and societies such as the International Commission on Glass ICG underline further that their expert opinion is increasingly getting attention. Inter alia and in the report period Prof. Ana Candida Rodrigues has been elected as the Chair of the Technical Committee 23: Education. Extremely positive in my opinion is their continuous diffusion of basic and glass science to students, professionals and the public. Certainly, a highlight of CeRTEV's professional qualification strategies was the 2nd Glass Technology Course August, 20-25th, 2018 where teachers were trained in the technical course of glass production.

Innovation and Technology Transfer

Also CeRTEV stood out in activities to bring science to business approach. With respect to biomaterial processing, the spin-off company VETRA should be especially noted. VETRA's core competencies in patents and products for clinical applications have been successfully developed in 2018.

In summa, the achievements of CeRTEV in all three areas are continuously outstanding and I would like congratulate the PIs for the hard work to keep this very high level of excellence in 2018.

June 24, 2019

TU Clausthal - Institut für Nichtmetallische Werkstoffe – Professur für Glas und Glastechnologie

Prof. Dr.-Ing. habil. Joachim Deubener 38678 Clausthal-Zellerfeld joachim.deubener@tu-clausthal.de

Prof. Dusan Galusek

As a member of the International advisory board of the CERTEV, I familiarized myself with the document sent to me by prof. Edgar D. Zanotto, the Centre's director. Based on these I came to the following conclusions:

1. The research activities of the Centre are anchored in deep theoretical understanding of glassy state of matter. They are characteristic by the use of modern theory-based methods and modelling with the use of artificial intelligence for data mining, leading to new quality of obtained results.

2. The expertise of principle investigators in the Centre covers all relevant aspects of glass research, especially those, related to investigation structure of glass by various instrumentation methods, relation between glass structure and properties, modelling, and various aspects of glass nucleation, crystallization and crystal growth.

3. The report documents a significant number of scientific outputs (approx. 100 peer reviewed scientific papers in the reported timeframe), but with strong focus on application oriented research in five different areas ranging from structural glasses to catalytic systems.

4. CeRTEV is involved in an impressive number of educational and outreach activities, including:

a. training of 40 students in collaboration with the Paula Souza Center, Abividro and the glass company Nadir Figueiredo,

b. activities aimed at the youngest generation (children of age 3-12 years old),

c. various workshops, meetings, lectures, public media outputs, and other dissemination activities

5. CeRTEV aimes at establishment of cooperation agreement and licensing of new technologies, as well as support of nuclei of spin-offs.

Recommendations for the following reporting period:

1. Apart from a list of scientific visitors, I found little mention on international research collaborations and received funding from international grant schemes. In the future, I therefore recommend stronger focus on formalized international collaborations with research establishments of similar research interests, attempting to achieve additional funding from funding agencies outside Brazil.

Dusan Galusek, Prof., DSc. FunGlass director

Dr. Vladimir M. Fokin

Vavilov State Optical Institute, Russian Fed

The present report figuratively says that glass is the eye of science. This successful expression can be used for another statement - fundamental science is the eyes of applied science! Building bridges between fundamental and applied sciences is a vital and extremely difficult task. Solving this problem requires high-level specialists who are experts in both areas. Since glass, which is an amorphous state of matter, is of both academic and practical importance, the above mentioned statement is directly relevant to it. The Center of Research, Technology, and Education in Vitreous Materials (CeRTEV) united specialists from three universities in charge of both traditional and modern research methods. I have known many of them for decades. The long duration of the project makes it possible to solve complex problems concomitantly, both fundamental and applied tasks. This report is impressive in the number of completed and published researches. The optimal ratio between fundamental and applied research It should be noted. In spite of this fact, that the papers listed in the report were published just recently, they are already well cited (an average of 17 citations / publication). That is, they found fast response in the scientific community. In conclusion, I want to congratulate the *CeRTEV team for the excellent results of intensive work.*

Prof. Richard K. Brow

I have reviewed the CeRTEV Report (#5, 2017-2018), and here are my comments and recommendations. I'll be happy to provide additional details, as you need them.

1. We have come to expect a world-class level of glass science from CeRTEV, and this report certainly fulfills that expectation. In particular, fundamental studies of the nature of glass and behaviors of glass-forming liquids will find their way into textbooks and classrooms for many years to come.

*Recommendation: CeRTEV might expand its computational/modeling portfolio into the areas of data mining and machine learning, to expand research influence in areas like composition-structure-property relationships, and to provide new tools for industrial partners.

2. There are some exciting technological advances coming from CeRTEV, including novel materials for biomedical applications and for fast-ion transport. I like the connection of the former work to the spin-off company (Vetra High Tech Ceramic Products), and believe this could be a model for other CeRTEV technologies.

*Recommendation: CeRTEV invests more time/resources in tech transfer/innovation activities to spin-off new companies and demonstrate to funding agencies the economic impact of the organization. What are the most mature technologies (gahnite transparent glass-ceramics? Na-ion conducting materials?) that could be developed into the next Biosilicate product?

3. The education/outreach activities are outstanding, with a wide range of products aimed at a diverse audience, from school children to glass professionals. Of particular note are the collection of "Wikividros" that should receive much broader publicity. CeRTEV should also be complimented for developing the outreach/training sessions for industry, and the organization of the University-Industry Workshop on Glass Materials.

*Recommendation: obtain testimonials from Brazilian glass manufacturers about the usefulness/utility of these training sessions to demonstrate to funding agencies the impact of CeRTEV on industry.

*Consider developing English versions of some of the educational products (e.g., the Glass Comics) for wider impact of CeRTEV activities.

Richard K. Brow

Curators' Distinguished Professor, Materials Science & Engineering Interim Director, Center for Biomedical Research Missouri University of Science & Technology Rolla, MO 65409

Dr. Jean-Luc Adam

CeRTEV is undoubtedly a center of excellence recognized worldwide for its outstanding research in glass science, especially in the domains of structural reinforcement materials for architecture and construction, bioactive glasses and glassceramics, fast ion-conducting materials for energy technologies, photonic glasses and glass-ceramics, and catalytically active systems. The Center has developed a very original and high-level research that combines both fundamental and applicationoriented studies. The number of scientific papers is very high (more than 100 articles in 2017-2018), most of them being published in very good journals dedicated to glass or material sciences. A good indicator of the original character of the work is the number of patents obtained by CERTEV every year, 4 patents for instance in the last two years in the field of bioglasses.

The international recognition is well accounted for by the very high number of oral presentations, and especially invited lectures (27 in 2017-2018), delivered by several CeRTEV members in high-level international conferences.

The attractivity of CeRTEV is excellent, as shown by the large number of postdocs involved in research projects (24 in 2017-2018). CeRTEV is also extremely effective in the education of new doctors in material science with 28 PhD either defended or in progress in that same period.

Also, CeRTEV develops an impressive strategy in promoting science among the society, especially with the development of professional qualifications in glass science and technology, and with the diffusion of basics of glass science into the public, including young people. The implication of CeRTEV scientists in the organization of international conferences is also outstanding.

In conclusion, CERTEV is among the very few glass research and education centers that are well-identified and recognized at the international level, thanks to its excellent research and promotion of science. Rennes, June 25th, 2019 Dr. Jean-Luc Adam, CNRS Research Director Phone : 33 (0)2 23 23 62 62 <u>jean-luc.adam@univ-rennes1.fr</u>

Prof. Christian Rüssel

Otto-Schott-Institute, Jena, Germany

Concerning the 5th report (2017-2018) of the Center for Research, Technology and Education in Vitreous Materials, CeRTEV, I would like to express the following:

Since its establishment, CeRTEV has done an impressive piece of work focused on both glasses and glass-ceramics. For me it was a surprise, that also new techniques, such as molecular dynamics and other simulation techniques have been utilized to study nucleation of glass. From my point of view, these techniques should widely complement the classical nucleation theory and clarify pre-nucleation phenomena.

The performed work is widespread and includes materials for a large variety of applications, such as biomaterials, high strength materials, ion conductive materials for energy storage, or materials for various photonic applications. In the past few years, research on new materials properties was done with increasing intensity. All this was performed with great success and complemented by theoretical studies especially (but not only) with respect to crystallization.

This resulted in an impressive number of publications in excellent international journals and even more in a very large number of conference contributions, many of them as invited lectures. Research activities were always combined with teaching activities, not only for PhD students but also for any other types of students and especially focused on glass research and fabrication of glass.

In summary, the activities of CeRTEV give an increasingly valuable contribution to glass science and to a general understanding of glassy materials. Moreover, also in combination with the student education, also a social impact is expected which, last not least, might result in a widening of the industrial production of glassy materials in Brazil, not only of everyday products, but also of a large variety of newly developed high tech products.

Altogether, I see CeRTEV research and education activities as great success.

Christian Rüssel Dr. rer. nat. Dr. Ing-habil Dr. h.c.

> Markus Rampf Schaan, 06/27/2019

The present report summarizes the impressive multitude of activities of the Center of Research, Technology, and Education in Vitreous Materials (CeRTEV). The activities and research is well organized and aligned following a clear strategy that covers traditional as well as the most emerging and high potential future fields of applications for glasses and glass-ceramics. The comprehensive and well respected competences of the CeRTEV in fundamental glass and glass-ceramics research, in particular the expertise in the investigation of glass-structure and crystallization, provides a sound base for this research strategy.

The quality and extent of the Center's activities in cutting-edge glass and glassceramic research reflects in the high number of original research and review papers published in well established scientific journals as well as the many contributions to international conferences.

Besides the very good scientific output, the efforts of the CeRTEV put into the recruiting and education of students and young academics (Education and Outreach) has to be highlighted. The Center, thereby, demonstrates social responsibility and contributes to a positive progress of society in Brazil.

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