

1. Fapesp form (attached file)

2. Cover page

Center for Research, Technology and Education in Vitreous Materials – CeRTEV
(www.certeve.ufscar.br)

Director: Edgar Dutra Zanotto
Universidade Federal de São Carlos / Departamento de Engenharia de Materiais / Laboratório de
Materiais Vítreos (lamav.weebly.com)

Edgar Dutra Zanotto – UFSCar: *Nucleation, crystal growth, crystallization and glass-ceramics – Director*
<http://lattes.cnpq.br/1055167132036400>

Hellmut Eckert - USP, São Carlos: *Structure, NMR methods - Vice-diretor*
<http://lattes.cnpq.br/7357691451348243>

Eduardo Bellini Ferreira - USP, São Carlos: *Nucleation, crystal growth, crystallization and glass-ceramics - Coordenador de Tecnologia e Inovação*
<http://lattes.cnpq.br/7703580367293028>

Ana Cândida Martins Rodrigues – UFSCar: *Electrical properties, ionic conducting glasses and glass-ceramics - Coordenador de Educação e Difusão do Conhecimento*
<http://lattes.cnpq.br/4499231813051400>

Leandro Innocentini Lopes de Faria – UFSCar–Gestor
<http://lattes.cnpq.br/0767710394930118>

José Fabián Schneider - USP, São Carlos: *Structure, NMR methods - Pesquisador Principal*
<http://lattes.cnpq.br/7617205350746681>

Andrea Simone Stucchi de Camargo Alvarez Bernardez - USP, São Carlos: *Optical properties, luminescence - Pesquisador Principal*
<http://lattes.cnpq.br/5990189383563490>

Marcelo Nalin - UNESP, Araraquara: *Optical and chemical properties - Pesquisador Principal*
<http://lattes.cnpq.br/3349586880746735>

Oscar Peitl – UFSCar: *Bio active glasses and glass-ceramics - Pesquisador Associado*
<http://lattes.cnpq.br/3007441705652783>

José Pedro Rino – UFSCar: *Molecular dynamics simulations - Pesquisador Associado*
<http://lattes.cnpq.br/6801067322823031>

Claudio José Magon - USP, São Carlos: *EPR and ESR techniques, Pesquisador Associado*
<http://lattes.cnpq.br/2717187327982497>

José Pedro Donoso Gonzalez - USP, São Carlos: *EPR and ESR techniques, Pesquisador Associado*
<http://lattes.cnpq.br/2572300460729333>

Paulo Sergio Pizani - UFSCar: *Raman spectroscopy, Pesquisador Associado*
<http://lattes.cnpq.br/1038437165007849>

Valmor Roberto Mastelaro - USP, São Carlos: *Structure, EXFAS, XRD and laser crystallization - Pesquisador Associado*
<http://lattes.cnpq.br/4361220072322558>

Marcello Rubens Barsi Andreetta – UFSCar: *Laser crystallization, crystal growth techniques - Pesquisador Associado*
<http://lattes.cnpq.br/7904227795652627>

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3. Summary of the project objectives (max 2 pgs.).

Through fundamental research on structure-property relations, using complementary simulation, spectroscopic and functional characterization methods, we are developing new active glasses and glass-ceramics with promising applications. For that, the core group of the Center consists of 14 professors at USP, UFSCar and UNESP (located in São Carlos and Araraquara, within 30km from each other) who are experts in engineering, chemistry and physics of vitreous materials, glass crystallization and a wide range of structural and functional characterization techniques. They advise about 50 students and post-docs engaged in glass and GC research and are embedded in a large Brazilian and international network of collaborations.

We are researching and developing new active glasses and glass-ceramics presenting application-relevant functionalities, such as high mechanical strength and electrical conductivity, biological, optical or catalytic activity, and/or combinations of these properties. A fundamental understanding of these properties is sought on the basis of the structural organization of these materials on different length scales. To this end, we are applying state-of-the-art NMR, EPR, EXAFS and vibrational spectroscopies to characterize the local and medium-range order, as well as the full resolution range of optical and electron microscopies, XRD and microanalyses for elucidating nano- and microstructures. This comprehensive experimental approach is being complemented by molecular dynamics simulations. Using this experimental modeling strategy, we are further seeking a fundamental understanding of glass sintering and crystallization in terms of the mechanisms, thermodynamics and kinetics of viscous flow, as well as crystal nucleation and growth, enabling us to exercise control of these processes by developing appropriate forming process and thermal treatment protocols. In a concerted effort, the participating laboratories are jointly investigating a number of important benchmark systems, which are deemed particularly promising for applications either as structural reinforcement materials (dental and bio glass-ceramics), optical materials (laser glasses), materials for electrochemical energy storage devices (electrolytes, high-temperature seals), and catalytically active systems. Our research agenda is complemented by continuous education and outreach activities at different levels as well as by technology development and transfer. We intend CeRTEV to develop into a state-of-art center for research, innovation, and education in the field of glass science and glass ceramics.

The CeRTEV Education and Outreach strategies and plan of action are divided in two main groups: *the first* is focused on the development of professional qualifications in glass science and technology, while *the second one* is focused on the diffusion of both basic and glass science. Being aware of the lack of professional training courses dedicated to the glass industry, which impinges upon its development, we consider it a high priority to remedy this situation. To this end, we are developing a comprehensive course, which will result in trained professionals for the glass industry. For this purpose, we are working with two professional organizations, the ABIVIDRO and the Paula Souza Center. Regarding our effort on diffusion, our strategy comprises multiple measures, which will be fully discussed later on in this report.

The research insights obtained from the CeRTEV activities will be channeled for generation of new technologies and patents, all the way to new products and production processes (“science to business approach”). We aim at the development of new or improved, patentable glass or glass-ceramic materials in each field of application above: 1) light armors (for use in airplanes, cars and individuals) and tougher monolithic glass-ceramics for dental restoration. We will work closely with some companies, such as Vitrovita and Cellmat; 2) macroporous and hierarchically ordered scaffolds, fibers, small monolithic parts and powders with increased osteoinductive activities, combined with the ability for targeted drug delivery for bone and tissue repair. Our industrial collaboration network in this area also includes Vitrovita, Vetra and DMC; 3) fast-conducting solid electrolytes for lithium ion batteries. Lithium ion cells in which these electrolytes are being implemented will be developed in São Carlos and tested in collaboration with the Münster Electrochemical Energy Technology center in Germany, a joint academic and industrial platform dedicated to the development of high-energy and high-power lithium ion batteries. We also aim at designing new glass-ceramic seals for fuel cell applications. Brazilian giants Petrobras and Itaipu are interested in these materials; 4) solid state lasing materials with enhanced emission characteristics. We intend to use our conceptual understanding and research expertise in crystallization and design for developing a novel application of transparent glass-ceramics.

4. Progress in the period related to the references of item (8) (max 20 pgs).

RESEARCH PROGRESS

Overview

The Center of Research, Technology, and Education in Vitreous Materials (CeRTEV) comprises 14 principal investigators and their co-workers the Federal University of Sao Carlos (UFSCar), the University of Sao Paulo (USP), (both located in São Carlos) and the State University of Sao Paulo (UNESP, located 30 km away in Araraquara). The principal investigators heading these groups are experts in vitreous materials, their crystallization and in a wide range of structural and functional characterization techniques. They advise about 50 graduate students and post-docs engaging in glass and glass-ceramic research, and are embedded in a large Brazilian and international collaboration network. Many of them have already collaborated with each other. As part of the joint CeRTEV research agenda, these groups work together to develop new active glasses and glass-ceramics, presenting application-relevant functionalities such as high mechanical strength, electrical conductivity, biological, optical or catalytic activity, and/or combinations of these properties. The synthesis efforts, which use both classical design strategies based on glass synthesis and controlled annealing as well as modern sol-gel-based self-assembly methods, are combined with detailed fundamental research aiming at an understanding of (a) how composition and microstructure control the structural and dynamical properties of glass-ceramics and (b) how the latter relate to macroscopic physical and functional properties.

The principal issues concerning this subject matter have been comprehensively discussed in a recent two-part review article [1]. They include the effects of liquid phase separation on crystal nucleation, tests and development of models of crystal nucleation, growth, and overall crystallization, metastable phase formation, surface crystallization, glass stability against devitrification, glass-forming ability, correlations between the molecular structure and nucleation mechanisms, sintering with concurrent surface crystallization, and diffusional processes that control crystal growth. Despite significant advancement in the knowledge about several aspects of phase transformations in glasses, glass crystallization remains an open, rich field to be explored [1].

The research agenda of CeRTEV is sub-divided into five core areas, dedicated to the five principal application fields of glasses and glass ceramics: (1) *structural reinforcement materials* for architecture and construction, armor, as well as dental restoration, (2) *bioglasses and glass-ceramics* for bone healing and growth, (3) *ion-conducting materials* for applications in modern energy technologies, (4) *photonic glasses and glass-ceramics*, and (5) *catalytically active systems*. All these application areas benefit from fundamental research encompassing the development of general concepts regarding the structural description of glasses and the structural, kinetic and mechanistic aspects of the nucleation and crystal growth processes involved in the crystallization of glasses leading to glass-ceramics, as described in more detail below.

1. STRUCTURAL REINFORCEMENT MATERIALS

1.1. New Formulations for Armor, Architecture, and Construction

Because of their unique thermal stability and shock resistance glass-ceramics are ideally suited for applications as materials for *armor* and *restorative dentistry*. The intrinsic fracture toughness and flexural strengths of glass-ceramics originate from their uniform microstructures, i.e. narrow grain size distribution, special crystal shapes and lack of voids. Research at CeRTEV has been devoted to developing and testing new glass ceramic formulations based upon the quest for an improved understanding of their structures, crystallization, microstructures and the resulting properties.

We have developed a new $\text{Li}_2\text{O}-\text{Al}_2\text{O}_3-\text{SiO}_2$ (LAS) ultra-low expansion glass-ceramic by non-isothermal sintering with concurrent crystallization. The optimum sintering conditions were $30^\circ\text{C}/\text{min}$ with a maximum temperature of 1000°C . The best sintered material reaches 98% of the theoretical density of the parent glass and has an extremely low linear thermal expansion coefficient ($0.02 \times 10^{-6}/^\circ\text{C}$) in the temperature range of $40^\circ\text{C}-500^\circ\text{C}$. This value is lower than that of the commercial glass-ceramic Ceran[®] that is produced by the traditional ceramization method. The sintered glass-ceramic presents a four-point bending strength of 92 ± 15 MPa, which is similar to that of Ceran[®] (98 ± 6 MPa), in spite of the 2% porosity. It is white opaque and does not have

significant infrared transmission. The maximum use temperature is 600°C [2]. It has a hardness of $H_{IT}=8.3\pm 0.4$ GPa and an elastic modulus of $E_{IT}=79\pm 2$ GPa, compared to $H_{IT}=9.1\pm 0.2$ GPa and $E_{IT}=85\pm 1$ GPa for Ceran. Tribological tests in dry conditions show lower wear rates than Ceran. Under wet conditions both materials have lower friction coefficients than in dry conditions, but wear rates are higher. We suggest that this new sintered GC could be an alternative, suitable material for cooktops [3].

1.2. Mechanistic Studies

A comprehensive mechanistic study has been carried out on non-stoichiometric glasses of the $\text{Li}_2\text{O} \cdot \text{SiO}_2\text{-CaO} \cdot \text{SiO}_2$ joint at deep undercooling [4]. Two distinct stages have been identified: In the first stage, lithium metasilicate (LS) crystals are formed. In the second stage, after a considerable delay, it is supplemented by the evolution of a calcium metasilicate (CS) phase. The analysis of the evolution of the residual liquid composition and its effect on the crystallization process revealed a novel phenomenon. The formation of LS crystals in the first stage of the process leads to the establishment of a transient equilibrium between the residual liquid and the LS-crystal phase. As a result, LS crystal growth is temporarily arrested. This termination of LS crystal growth occurs when the composition of the residual liquid reaches that of the metastable liquidus for LS at given temperature and pressure. The growth of LS crystals is resumed only in the second stage of the process when the CS crystals form. The evolution of the CS-crystal phase changes the composition of the residual liquid and shifts it away from the composition corresponding to the metastable liquidus. As a result, the LS crystals again become capable of further growth. The above crystallization pathway is expected to be a general phenomenon in phase formation in multi-component systems with different mobilities of the components determining the kinetics of formation of the different phases [4]. A variation of the glass composition from the eutectic (26.5 mol% Li_2O) towards lithium metasilicate (50 mol% Li_2O) results in a sharp increase of the internal nucleation rate of LS crystals, whereas the growth rates increase only weakly. This strong increase of the nucleation rate is primarily caused by a decrease of the thermodynamic barrier for nucleation - due to an increase of the thermodynamic driving force for crystallization and a decrease of the nucleus/liquid interfacial energy - as the glass composition approaches the crystal composition [5].

1.3. New Characterization Methods

Structural investigations on glasses and glass ceramics benefit greatly from new methodologies and techniques for the acquisition of structural information at the atomic/molecular scale. Within CeRTEV, technique-oriented research of this kind is under active development. One subject of key interest concerns the accurate measurement of nucleation rates. It had been previously proposed that this measurement can be done by evaluating the areas under the differential scanning calorimetry (DSC) crystallization peaks of partially crystallized glass samples. We have explored this method in detail for lithium disilicate glass, a material of great fundamental interest and technological importance. When comparing the results with those obtained by the more established methods of optical microscopy, a substantial discrepancy is noted which is attributed to the formation of new nuclei during the heating and cooling paths of the DSC runs. In addition there may be surface crystallization effects that are not taken into account in the DSC expressions [6]. In principle, the rate of crystallization in lithium disilicate glass ceramics can also be measured by ^{29}Si solid state nuclear magnetic resonance (NMR) spectroscopy, as the signals of the crystalline and glassy fractions are clearly distinguishable. Unfortunately, however, this approach is not feasible in practice as the ^{29}Si spin-lattice relaxation times are extremely long, thereby complicating rigorously quantitative applications. It could be shown, however, that greatly enhanced ^{29}Si NMR signals can be obtained via $^7\text{Li}\text{-}^{29}\text{Si}$ cross-polarization and that this method can be calibrated to yield quantitative nucleation rates consistent with those determined by optical microscopy and x-ray powder diffraction [7]. Recently, our experimental work has been complemented by molecular dynamics simulations, which have been used to reveal details of the diffusion mechanism in lithium disilicate melts [8]. Having established appropriate methodology, we will extend these works to explore details of nucleation and crystal growth processes in this material. A new solid state NMR technique has also been developed for measuring homo-nuclear dipole-dipole interactions for the analysis of distance distributions in glasses [8]. The method which is given the acronym DQ-DRENAR (**D**ouble-**Q**uantum-based **D**ipolar **R**e-coupling **E**ffects **N**uclear **A**lignment **R**eduction) measures the rate with which double quantum coherences are being stimulated. This rate depends on the nuclear spin-spin coupling strengths, which in turn depend on the inter-nuclear distances. The method has been successfully validated for $^{31}\text{P}\text{-}^{31}\text{P}$ distance determinations of numerous crystalline model compounds representing a wide range of dipolar coupling strengths and also applied to various glassy systems [9]. Important new progress has also been made on the data processing side of NMR and EPR results [10]. As an alternative to the Fourier Transform, the Krylov Basis Diagonalization Method (KBDM) has been used as an alternative analysis method for the processing of time domain signals acquired by pulse NMR and EPR signals. In this numerical procedure the signals are fitted as a sum of exponentially damped sinusoids.

Our results lead to the conclusion that the KBDM can be successfully applied, mainly because it is not influenced by truncation or phase anomalies that sometimes affect the Fourier transform spectra [10].

2. BIOACTIVE GLASSES AND CERAMICS

2.1. Compositional Effects on Bioactivity

Research at CeRTEV on bioactive glasses focuses on the continuing improvement of osteoconductive and osteoinductive materials for stimulating bone healing and growth, by developing and testing new bioactive formulations and composites and comparing their performances to the “golden standard” glass denoted “45S5” developed by Professor Hench and co-workers.

The use of different phosphate precursors for bioactive CaO-SiO₂-P₂O₅ glasses, while requiring an adaptation of the sol-gel synthesis and calcination protocols, does not affect the bioactivity of the final products [11]. In contrast, magnesium is known to have strong effects, even though its functional properties for osteoconduction and –induction are subject to some controversy in the literature. This controversy is related to the question of whether MgO acts as a network former or as a network modifier species. We have conducted a systematic in-vitro study of the effect of calcium substitution by magnesium in 45S5 glass [12]. While this substitution leads to glasses with significantly enhanced stability against crystallization, the dissolution kinetics of the glass are essentially unaltered, indicating that in this glass system MgO does not act as a network former or intermediate oxide. Furthermore, FTIR and solid state ³¹P and ¹H MAS-NMR consistently indicate that partial replacement of CaO by MgO in the bio-glass formulation does not influence the rate at which the initial amorphous calcium phosphate (ACP) layer is precipitated when the glass is exposed to SBF. It greatly reduces, however, the rate of conversion of this precursor phase to the crystalline hydroxycarbonate apatite (HCA)-layer [12].

We have further developed and tested a new biomaterial named “Biosilicate”, representing a group of fully crystallized glass-ceramics of the Na₂O-CaO-SiO₂-P₂O₅ system [13-17]. The carbonated hydroxyapatite (HCA) layer is formed in less than 24 hours of exposure to SBF, suggesting excellent bioactivity. In vitro studies with osteoblastic cells reveal further that this ceramic supports significantly larger areas of calcified matrix compared to 45S5 Bioglass, indicating its potential to promote enhancement of in vitro bone-like tissue formation in osteogenic cell cultures [13]. The biocompatibility of Biosilicate® scaffolds was evaluated by means of histopathological, cytotoxicity, and genotoxicity analysis. In the histopathology analysis, we observed a foreign body reaction, characterized by the presence of granulation tissue after 7 days of implantation of the biomaterial into male rats, and fibrosis connective tissue and multinucleated giant cells for longer periods. In the cytotoxicity analysis, extracts from the biomaterial did not inhibit the proliferation of osteoblasts and fibroblasts, and relatively low concentrations (12.5% and 25%) stimulated the proliferation of both cell types after 72 and 120 h. The analysis of genotoxicity showed that Biosilicate® did not induce DNA damage in both lineages tested in all periods [14]. All of these studies reveal that the material is biocompatible, presents excellent bioactive properties, and is effective to stimulate the deposition of newly formed bone in animal models, thus suggesting great promise for bone regeneration applications [15-17].

2.2. New Bioactive Glass Formulations and Composites

Biosilicate-based scaffolds possessing the main requirements for use in bone tissue engineering (95% porosity, 200-500 μm pore size) were also successfully produced by the foam replica technique [18]. To increase the mechanical competence of the scaffolds gelatine coating was used as a simple approach, resulting in significantly increased compressive strengths (i.e. 0.80 ± 0.05 MPa of coated versus 0.06 ± 0.01 MPa of uncoated scaffolds), without interfering with the porosity and bioactive properties of the material. Based on these results, the combination of Biosilicate® glass-ceramic and gelatine is attractive for producing novel scaffolds for bone tissue engineering [18].

Bioglasses have also been successfully introduced as new additives to calcium phosphate cements (CPCs), which are used as an alternative to biological grafts due to their excellent osteoconductive properties. Although the degradation of CPCs can be improved by using poly(D,L-lactic-co-glycolic) acid (PLGA) microspheres as porogens, the biological performance of CPC/PLGA composites is insufficient to stimulate bone healing in large bone defects. Owing to the unique ability of bioactive glasses (BGs) to bond to living bone the incorporation of BGs into calcium phosphate cement (CPC) was tested as an approach to improve the biological performance of CPC. To this end, the setting properties, in vitro degradation behavior, and morphological characteristics of CPC/BG and CPC/PLGA/BG composites have been studied in detail. The results indicate that BG can be

successfully introduced into CPC and CPC/PLGA without exceeding the setting time beyond clinically acceptable values. All injectable composites containing BG that were studied had suitable handling properties and specifically CPC/PLGA/BG showed an increased rate of mass loss [19]. The in vivo performance of BG supplemented CPC, either pure or supplemented with PLGA microparticles, was evaluated via both ectopic and orthotopic implantation models in rats [20]. Upon ectopic implantation, incorporation of BG into CPC improved the soft tissue response by improving capsule and interface quality. Additionally, the incorporation of BG into CPC and CPC/PLGA showed 1.8- and 4.7-fold higher degradation and 2.2- and 1.3-fold higher bone formation in a femoral condyle defect in rats compared to pure CPC and CPC/PLGA, respectively. Our results highlight the potential of BG to be used as an additive to CPC to improve the biological performance for bone regeneration applications.

3. GLASS-CERAMICS FOR APPLICATIONS IN MODERN ENERGY TECHNOLOGIES.

Recently glass-ceramics have shown significant promise for applications as solid electrolytes in high energy storage devices. The highest lithium ion conductivities in the solid state are generally encountered in crystalline compounds with highly disordered cation sub-lattices, termed *super ionic crystals*. Nevertheless, ion conducting glasses are often preferred in practice as they do not suffer from grain boundary effects and form more homogeneous interfaces with the anode and cathode compartments of a solid state electrochemical cell. The favorable features of both the crystalline and the glassy state can be combined using ion conducting glass-ceramics, and numerous promising systems presenting electrical conductivities in excess of $10^{-3} (\Omega \cdot \text{cm})^{-1}$ at room temperature exist. The CeRTEV research agenda focuses on the further development of such systems, based on a solid understanding of composition – structure – performance relationships. Rather than attempting the development of completely new compositions, we are seeking a better understanding of what the limitations of the current *lead-materials* are and how they can be overcome.

3.1. Composition/Structure Relations in NASICON-type Glass Ceramics.

One particularly attractive system is based on the crystallization of precursor glasses in the highly conductive NASICON structure. These systems are based on the $\text{LiTi}_2(\text{PO}_4)_3$ composition, and their ionic conductivity can be enhanced further by aliovalent ion substitutions, e.g. Al^{3+} on Ti^{4+} and/or Si^{4+} or Ge^{4+} on P^{5+} sites, resulting in rather complex compositions denoted as $\text{Li}_{1+x+y}\text{Ti}_{2-x}\text{Al}_x\text{Si}_y\text{P}_{3-y}\text{O}_{12}$ (LTAP). Recently, these materials have shown promise as solid electrolytes in lithium/air batteries offering potential energy densities of up to 11140 kWh/kg. As the composition and microstructure optimization of these materials is still largely an empirical effort, there is a great need for developing a detailed fundamental understanding of the composition – performance relationship on the basis of quantitative information regarding both the structure and the dynamics of these systems.

The crystallization kinetics of a glass with the composition $\text{Li}_{1.5}\text{Al}_{0.5}\text{Ge}_{1.5}(\text{PO}_4)_3$ have been studied in detail using differential scanning calorimetry [21]. Using Ligeró's and Kissinger's methods the activation energy of crystallization, was determined to be near 400 kJ/mol. The Avrami coefficient was found to be $n = 3.0$, consistent with the observation of predominant volume (as opposed to surface) crystallization [21]. The crystal-to-glass transition can also be quantitatively monitored by ^{31}P solid state NMR, and the fraction of crystalline material has been correlated with ionic conductivity data. These studies suggest a threshold phenomenon near crystallization degrees as low as 10% [22]. The structural aspects of the glass-to-crystal transition have been examined by complementary multinuclear solid state nuclear magnetic single and double-resonance experiments. While the crystalline materials are based on octahedral germanium and aluminum coordination, the glasses show aluminum in four-, five- and six-coordination. Despite the significantly larger degree of disorder concerning the local coordination of germanium and aluminum, dipolar solid state NMR studies clearly indicate that the medium range structures in the glassy and crystalline states are comparable, indicating the dominance of P-O-Al and P-O-Ge over P-O-P and Al-O-Ge linkages [23].

3.2. Non-linear Composition/Property Relations in Ion-conducting Glasses.

A general approach in tailoring the performance of glasses to specific applications is based on fine-tuning the chemical composition. When this general principle is applied to ion-conducting glasses one frequently encounters strikingly non-linear changes in physical properties (such as the ionic conductivity). One prominent example known as the “*mixed alkali effect*” has been discussed in the literature for more than a century. Similar non-linear phenomena are often encountered when two or more network former oxides are used in the glass formulation (“*mixed network former effect*”) or when different kinds of anions are involved (“*mixed anion*”).

effect”). For making optimal use of such dependences in compositional design, a detailed structural understanding is sought on the basis of advanced solid-state NMR methods.

3.2.1. Mixed Network Former Effects.

With the above-stated objective the structure of glasses in the system $(M_2O)_{0.33}[(Ge_2O_4)_x(P_2O_5)_{1-x}]_{0.67}$ ($M = Na, K$) has been studied by ^{31}P and ^{23}Na high-resolution and dipolar solid state nuclear magnetic resonance (NMR) techniques, O-1s X-ray photoelectron spectroscopy, and Raman spectroscopy [24]. Using an iterative fitting procedure, a quantitative structural model has been developed, providing a detailed description of network connectivities, network modification processes, and spatial cation distributions. Formation of hetero-atomic P-O-Ge linkages is generally preferred over homo-atomic P-O-P and Ge-O-Ge linkages. The phosphate component is preferentially modified by the cations. Consequently the local coordination of the cations is dominated by phosphorus, which has been quantified by dipolar NMR experiments. The joint interpretation of all of the experimental data offers indirect evidence for the formation of higher germanium coordination states in this glass system.

3.2.2. Mixed-Modifier Effects

Multinuclear solid state NMR has also been used to explore the structural aspects of *mixed-cation effects* (MCE) in various metaphosphate glasses based on the cation combinations Cs-Li, Rb-Li, and Cs-Ag, exhibiting particularly large size mismatches [25]. The results are compared with those obtained in the Na-Ag metaphosphate series, which serves as a reference system, with minimized cation mismatch. The local coordination environments of the Ag^+ , Rb^+ and Cs^+ ions follow analogous compositional trends as previously observed in Na-based mixed-ion metaphosphate glasses: for a given cation species A, the average A-O distance shows an expansion/compression when this cation is replaced by a second species B with smaller/bigger ionic radius, respectively. This compositional differentiation of the structural sites for the mobile species may contribute to the MCE. Concerning the relative spatial distribution of the mobile ions, results from 7Li - ^{133}Cs spin echo double resonance (SEDOR) experiments indicate a random mixture of Cs and Li in Cs-Li metaphosphate glasses. In the Cs-Ag and Na-Ag glasses, ^{109}Ag spin-echo NMR reveals a progressive slowing down of the Ag^+ diffusion dynamics as this species is replaced by Cs^+ or Na^+ . The substitution by the bigger Cs^+ ion causes a strong reduction in Ag^+ mobility suggesting the existence of separated diffusion pathways for these cations. In contrast, substitution by the similarly-sized Na^+ causes a much weaker mobility reduction consistent with the existence of Ag-Na cooperative hopping [25].

3.2.3. Mixed-anion Effects.

Mixed anion effects have been investigated on various silver ion conductive glasses [26]. In the $x AgI (1-x) AgPO_3$ system ($0 \leq x \leq 0.5$), ionic conductivity is due to the motion of silver ions in the glass. Experimentally an increase by more than four orders of magnitude is observed when x varies from 0 to 0.5, although the number of silver cations remains constant. The ionic conductivity (σ_+) can be expressed as $\sigma_+ = n_+ e \mu_+$. As previous studies had shown that the charge carrier mobility (μ_+) is independent of the glass composition, within the framework of the weak electrolyte theory the observed effect must be attributed to a corresponding increase in the number of effective charge carriers (n_+) [26]. The strong concentration dependence observed in such glasses has been frequently related to AgI clustering phenomena. We have explored this clustering issue by modern solid state NMR techniques for a new, highly conductive glass system accessible by roller-quenching of $(Ag_3PO_4)_x(AgI)_{1-x}$ melts ($0.15 \leq x \leq 0.50$) [27]. The composition dependences of the ^{109}Ag and ^{31}P chemical shifts suggest a statistical distribution of the phosphate and iodide anions. This conclusion is quantitatively confirmed by DQ-DRENAR [9] experiments, which numerically prove a random spatial distribution of the phosphate anions. Altogether these results give the final answer to a long-standing debate on the structure of AgI-based glasses, proving the absence of previously postulated silver iodide cluster domains [27].

4. GLASS-CERAMICS FOR PHOTONIC APPLICATIONS.

The development of new optical materials based on inorganic hosts doped with luminescent rare-earth ions or complexes is an active area of current materials research. In this connection CeRTEV's activities pursue a three-pronged approach: (1) the development of new glass and glass ceramic formulations doped with luminescent rare-earth emitter ions, (2) the synthesis and utilization of luminescent glasses doped with metal nanoparticles and (3) the immobilization of organic luminophores and rare-earth or transition metal ion complexes in porous hosts using various chemical strategies. To facilitate the design of materials with optimized emission properties,

detailed structural information at the atomic level is essential, regarding the local bonding environment (siting) of the luminophores, their second-nearest coordination spheres, and their extent of local clustering or molecular aggregation, as well as the distribution over separate micro- or nanophases in composite materials. For this effort, CeRTEV research aims at detailed correlations of photophysical properties (emission intensities, excited state lifetimes and quantum yields) with the structural characteristics elucidated by solid state NMR and EPR techniques.

4.1. New Formulations for Luminescent Rare-Earth Doped Glasses and Glass-Ceramics

Inorganic glasses doped with luminescent rare-earth ions are still at the focus of much attention, not only for laser applications, but also as constituents of several other devices such as amplifiers, detectors, sensors, etc. This interest stems from the compositional and fabrication flexibility of glassy materials, and also their ability to incorporate much higher concentrations of dopants than crystals. Since binding of the RE ions to fluoride rather than oxide ions can dramatically improve their vibrational relaxation characteristics, resulting in longer excited-state lifetimes and larger quantum yields, fluoride-containing glasses have been attracting considerable interest. On the other hand, pure fluoride glasses suffer from poor mechanical and chemical stability and fiber drawing is difficult. If, on the other hand, a material can be designed such that the local environment of the rare earth species is dominated by fluoride ions, while the structural framework is stabilized by strong oxide linkages, such glasses (or glass-ceramics) can combine, in an ideal way, the low-phonon energy characteristics of pure fluoride hosts with the high mechanical strength and chemical stability of oxide-based glasses. For the development of high-power laser systems, high luminescent ion concentrations must be realized, while simultaneously maintaining a maximum degree of dispersion to prevent concentration quenching effects. We have developed a new fluorophosphate glass formulation in the compositional line $(30-x)\text{Al}(\text{PO}_3)_3-x\text{AlF}_3-25\text{BaF}_2-25\text{SrF}_2-(20-z)\text{YF}_3-z\text{YbF}_3$ ($0 \leq x \leq 20$; $0 \leq z \leq 5$) which shows considerable promise in this respect [28]. The characteristic improvement in hydrolytic stability and phonon energy of the glasses, as compared to their oxide analogues, result in long ${}^2\text{F}_{5/2}$ radiative lifetime values ($\tau_0 = 1.2$ ms) and high critical Yb^{3+} concentrations ($Q = 6.8 \times 10^{20}$ ions/cm³). Special attention has been devoted to the (non-) radiative decay processes, namely radiation trapping (RT), self-quenching (SQ), and cooperative luminescence (CL). Strong radiation trapping effects are observed, which can be favorably used to generate highly efficient energy upconversion in the blue, through Yb-Yb cooperative effects. A CL rate of 32 s^{-1} was realized for a typical pump power of ~ 100 mW. These characteristics suggest potential applications for blue emitting devices, as well as for infrared ones [28]. Detailed structure/property correlations of this system addressing the local environment of the RE ions in this glass system by nuclear magnetic resonance (NMR) and electron paramagnetic resonance (EPR) are currently under investigation [29].

Photo-thermo-refractive (PTR) glass is an optically transparent photosensitive oxide glass. Upon heating, the UV-exposed regions of this glass undergo copious crystallization of NaF nano-crystals giving rise to a permanent, localized refractive index change. But the unexposed parts of the glass also undergo some crystallization which causes unwanted light scattering. Holographic optical elements produced from PTR glass have been used in special laser systems. We have measured, for the first time, steady-state nucleation rates, nucleation time-lags and crystal growth rates for UV-unexposed PTR glass over a wide temperature range, from $T_g \sim 470$ °C up to 750 °C. A self-consistent description of these data is presented in the framework of classical nucleation theory using the interfacial free energy of the critical nuclei and the effective diffusion coefficient as adjustable parameters. The diffusivity calculated from crystallization kinetics and that estimated from viscous flow via the Stokes-Einstein-Eyring equation show a decoupling phenomenon [30].

4.2. Photonic Devices based on Metal Nanoparticle-Doped Glasses

Metal nanoparticle doping is known to dramatically increase absorbance and emission intensity of rare-earth doped glasses. The creation of such nanoparticles within the glassy matrix and their transformation during annealing and ceramization, however, still presents substantial challenges. Detailed studies have been carried out on a series of glasses, doped with Ag- and Cu- nanoparticles, varying the chemical nature of the precursor [31]. We have further prepared heavy metal oxide glasses containing metallic copper nanoparticles with promising nonlinear optical properties as determined by Z-scan and pump-probe measurements using femtosecond laser pulses [32]. For the wavelengths within the plasmon band, we observe saturable absorption and response times of 2.3 ps. For the other regions of the spectrum, reverse saturable absorption and lifetimes shorter than 200 fs were verified. The nonlinear refractive index is about $2.0 \times 10^{-19} \text{ m}^2/\text{W}$ from the visible to the telecom region, thus presenting an enhancement effect at wavelengths near the plasmon and Cu^{+2} d-d band [32].

One of the most promising new technologies for nanoparticle creation is femtosecond laser processing of suitably composed precursor glasses. At CeRTEV we have used this method to induce Cu and Ag nanoparticle formation in the bulk of borate and borosilicate glasses, which can be applied for a new generation of waveguides. Also 3D polymeric structures have been fabricated by two-photon polymerization, containing Au and ZnO nanostructures with intense two-photon fluorescent properties [33]. Finally, hexagonal Photonic Crystal (2D-HPC) layers, with a linear waveguide, have been prepared in erbium doped $\text{GeO}_2\text{-Bi}_2\text{O}_3\text{-PbO-TiO}_2$ glassy films, by combining the techniques of holographic recording and femtosecond (fs) laser micromachining [34]. The 2D-HPC is recorded holographically in a photoresist film coated on a glass substrate by exposing the sample to the same interference pattern twice and rotating the sample of 60° between the exposures. After the development a two dimensional hexagonal array of photoresist columns remains on the glass substrate. The recording of the waveguide is made by a fs laser micromachining system focused at the sample surface. The laser spot produces the ablation of the photoresist columns generating a defect line in the periodic hexagonal array. After the recording of the photoresist template, the erbium doped $\text{GeO}_2\text{-Bi}_2\text{O}_3\text{-PbO-TiO}_2$ film is evaporated on the photoresist and finally the photoresist template is removed using acetone. The design of the geometrical parameters of the 2D-HPC is performed by calculation of the dispersion mode curves of the photonic crystal using a 2D finite element method. The proper geometrical parameters depend on both the refractive index of the glass film and thickness. Such parameters as well as the period of the 2D-HPC have been defined in order to obtain a photonic band gap in the region of erbium luminescence band. In such condition the erbium luminescence will propagate only through the waveguide [34,35]. Altogether, the results obtained so far suggest that femtosecond laser processing to fabricate glasses doped with metal or semiconductor nanostructures shows substantial promise for the creation of new optical sensors and photonic devices.

4.3. Luminescent Hybrid Materials Based on Rare-Earth Complexes in Porous Hosts.

The third group of active photonic materials studied within CeRTEV comprises inorganic-organic hybrid materials based on the incorporation of luminescent organic dyes or transition or rare-earth metal coordination compounds into inorganic host matrices. This work includes (a) the development of new luminophore molecules with higher quantum yields and excited state lifetimes, (b) the immobilization of such molecular emitters in suitable hosts, and (c) the application-relevant optimization of such hybrid materials by tailoring the intermolecular guest-host and guest-guest interactions.

4.3.1. New Emitters

We have synthesized and characterized a new nine-coordinate Eu^{3+} complex containing three tridentate ligands and exhibiting one of the highest emission quantum yields ($\Phi = 85\%$) so far reported [36]. Using ligand field theory (LFT) and semi-empirical calculations the energies of the $^7\text{F}_{JM}$ Stark levels of the ion were predicted with the aim to find the best geometry of the complex on the basis of matching experimental data. The results from the LFT analysis corroborate the existence of a nine-coordinate Eu^{3+} center and prove the transferability of the charge factors used in this theoretical model.

4.3.2. Emitter Immobilization Strategies

For the immobilization of luminescent complexes in suitable solid hosts, a variety of strategies are being employed at CeRTEV. These include (a) *wet impregnation* [37], (b) *co-assembly* [37], (c) *covalent attachment* [38] and (d) *ion exchange* processes [37,39]. For the immobilization of neutral nine-fold Eu complexes of the kind described above, the covalent attachment strategy has been successfully applied for binding the luminophore to the inner pore walls of the mesoporous silica host MCM-41 using the grafting method [38]. Guest-host binding is achieved through double functionalization of the host surface with organosilane reagents (hexamethyldisilazane, HMDS, and aminopropyltriethoxysilane, APTES) followed by reaction of the active amino sites of the APTES residue with the ligand 2,2'-bipyridyl-6,6'-dicarboxylic acid, subsequent addition of EuCl_3 solution and further addition of 2,2'-bipyridine-6 monocarboxylic acid ligand in the final reaction step. The covalently attached Eu complex displays promising emissive properties, even though the results suggest that it may be difficult to fully realize the nine-fold Eu coordination environment in this manner [38].

The *ion-exchange* method has been successfully used for the immobilization of a cationic bis-cyclometalated Ir(III) complex $[\text{Ir}(\text{dfptrBn})_2(\text{dmbpy})]^+$ ($\text{dfptrBn} = 1\text{-benzyl-4-(2,4-difluorophenyl)-1H-1,2,3-triazole}$; $\text{dmbpy} = 4,4'\text{-dimethyl-2,2'-bipyridine}$) into mesoporous sodium aluminosilicate sol-gel glasses [39]. The resulting hybrid material exhibits superior photophysical properties, such as increased photoluminescence lifetime values compared to dilute solutions. The influence of the chemical environment around the Ir(III)

complex upon its photophysical properties was rationalized on the basis of density functional theory (DFT) and time-dependent DFT (TDDFT) calculations. In low-polarity media ($\epsilon < 20$) the coupling between the cationic Ir(III) complex and the counterion appreciably affects its electronic structure [39].

The *co-assembly* strategy has been used to incorporate Rhodamine 6G (Rh6G) dye into pure (SiO_2) and phenyl-modified silica ($\text{Ph}_{0.17}\text{SiO}_{1.915}$) xerogels, prepared via sol-gel reaction using an ionic liquid as a catalytic agent. By this method the concentration of surface hydroxyl groups in the host can be nearly completely suppressed, resulting in superior emission properties of the incorporated dye. High quantum yield values (up to 87%) were observed, with no substantial decrease in efficiency with increasing dye concentration. At suitable Rh6G contents, all the final materials present laser action under 532 nm excitation from a Q-switched frequency doubled Nd:YAG laser. The phenyl silicate sample presents the highest laser photostability with a half-life of 6560 pulses, under 2 mJ/pulse pump power, and 10 Hz repetition rate [37]. Finally, amorphous DNA-biopolymer-based membranes have been explored as suitable hosts for the incorporation of luminescent Er^{3+} ions with the purpose of producing highly efficient emitting phosphors forelectrochromicdisplay devices. The materials exhibit high ionic conductivities, e.g. on the order of 10^{-5} Scm^{-1} for DNA_{10}Er -triflate and have an acceptable redox stability window (2 V). The optimization of these materials is currently conducted on the basis of detailed structural investigations using EPR and NMR spectroscopies [40,41].

5. CATALYTIC GLASSES AND GLASS-CERAMICS

At the present time, glass-ceramics have been explored very little for catalytic conversions of any kind. In general, catalyst design has been the chief objective and domain of self-assembly and supramolecular chemistry, resulting in zeolites, mesoporous and hierarchically structured materials, which are then functionalized for catalytic applications. While the use of such materials for catalytic biomass-to-fuel conversions has been amply documented in the literature at the present time no large-scale industrial plants utilizing zeolites or mesoporous catalysts are yet in operation within Brazil. The transport of heavy biomass molecules into catalyst pores is very cumbersome and severe mass transfer limitations should be expected. To be transformed the biomass requires a dispersant as reaction medium and catalyst materials with interconnected systems of very large pores (macropores). The generation and catalytic functionalization of such macroporous glass-ceramics and of hierarchically structured materials combining meso- and macroporosity is part of CeRTEV's research agenda. For generating macroporosity, we currently pursue sintering of powdered ceramic suspensions together with pore-forming agents on model stoichiometric glasses such as $2\text{MgO} \cdot 2\text{Al}_2\text{O}_3 \cdot 5\text{SiO}_2$ and $\text{Li}_2\text{O} \cdot 2\text{SiO}_2$, which are powdered and compacted with pore-precursor additives such as Ca alginate. The glass formulations are being modified with catalytically additives such as TiO_2 and metal nanoparticles (Au), giving these materials catalytic properties for conversion of plant biomass into chemicals of high industrial value [42].

Mesoporous glasses along the composition line $0.5\text{Al}_2\text{O}_3 \cdot x\text{SiO}_2$ ($1 \leq x \leq 6$) were prepared via a novel sol-gel route using tetraethylorthosilicate and aluminum lactate as precursors [43]. The structural evolution from solution to gel to glass is monitored by standard ^{27}Al and ^{29}Si nuclear magnetic resonance (NMR) spectroscopies, revealing important insights about molecular level mechanisms occurring at the various stages of glass formation. Following calcination at 650°C , average pore diameters of about 3 nm and surface areas near $500 \text{ m}^2/\text{g}$ have been realized. Advanced solid state NMR methods have been applied to probe the connectivity and the extent of compositional segregation in this system [44]. Overall the results indicate a higher degree of homogeneity than that of other silica-alumina preparations using different Al precursors. In the next step we will explore chemical strategies for functionalizing the inner pore surfaces with suitable agents for oxidation catalysis. For catalytic testing, we have designed a suitable reference system consisting of inorganic clay intercalated with a free nitroxide radical. The catalytic activity of this material has been evaluated using the oxidation of benzyl alcohol as a standard test reaction, furnishing us with data for comparison with the performance of corresponding macroporous ceramics [45]. A comprehensive strategy comprising a variety of complementary advanced solid state NMR experiments has been designed for structural characterization [45]. In conceptually related work, Cu(II) complexes have been intercalated into such clays, and the nature of the catalytically active species has been characterized by EPR spectroscopy [46]. Two-component Cu^{2+} EPR spectra are observed, indicating the coexistence of isolated Cu^{2+} with a well-resolved hyperfine structure and spin-spin exchanged Cu^{2+} dimers or clusters with an unresolved hyperfine structure. The interaction between the paramagnetic centers is mainly favored by two different phenomena: turbostratic disorder of clay sheets and segregation of the magnetic centers leading to interstratifications of layers [46]. Overall, the above-described investigations have put a powerful and comprehensive characterization strategy at our disposal. This will be helpful for uncovering important structure-function relationships in catalytically active macroporous ceramics.

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EDUCATION AND OUTREACH PROGRESS

Overview

The CeRTEV Education and Outreach strategies and plan of action are divided in two main groups: *Group A* focuses on the development of professional qualifications in glass science and technology, while *Group B* has as its main objectives the diffusion of basic and glass science. We will describe below the main actions taken in groups A and B, during this first year of CeRTEV's activities.

Group A: Development of professional qualification strategies in glass science and technology

Being aware of the lack of professional training courses dedicated to the glass industry, which impinges upon its development, we consider it a high priority to remedy this situation. To this end, we are developing a comprehensive course, which will result in trained professionals for the glass industry. For this purpose, we are closely working with two very important partners, the ABIVIDRO and the Paula Souza Center.

The ABIVIDRO (Associação Técnica Brasileira das Indústrias Automáticas de Vidro- Brazilian Association of Automated Glass Industry) comprises the ~20 most important companies in glass industry in Brazil, most of them located in the state of São Paulo (the CeRTEV state). Aside from the multinational giants, some of these companies are financed with Brazilian capital.

The Centro Paula Souza is an organization of the São Paulo State Government which now administrates 214 Technical Schools (ETECS) and 59 Faculties of Technology (FATECS) in 163 municipalities of the state of São Paulo. The ETECS assist more than 216,000 students in high schools and at the technical level. Also, FATECS has more than 64,000 students enrolled in technology-related undergraduate courses.

The CeRTEV team has organized several meetings with the two above institutions, whose outcomes can be summarized as follows. We first introduced our project to ABIVIDRO, which confirmed the lack and necessity of the creation of such technical courses dedicated to training personnel to glass industry. We then had a second meeting with ABIVIDRO and representatives of the Centro Paula Souza, where ABIVIDRO described all the benefits such technical courses could generate to the glass industry. In turn, the Paula Souza Center requested a description of the various technical positions the glass industry needs.

Subsequently, these descriptions were developed by CeRTEV and ABIVIDRO and presented to the Centro Paula Souza. To learn more about the specific needs involved two site visits with companies were scheduled. During the first one, the group visited a Brazilian Company, Nadir Figueiredo (Suzano, SP), Cebrace (Jacareí, SP) a joint-venture between Saint-Gobain and NSG (Japan) – the biggest producer of float glass in South America, and also NSG, ex-Pilkington (Caçapava, SP), a glass transformation company which fabricates laminated and tempered glass for the automotive industry. The second visit took place at Speed Temper, a medium - range Brazilian (family business) transformation enterprise. This company fabricates tempered and laminated glasses for building construction. It also makes beveled glasses and lapidified finishing. During these visits, the representatives of Centro Paula Souza talked with the technical staff who confirmed the total absence of official technical education. All technical training and education is being exclusively done in an *ad-hoc* manner “on the job”. Currently, a “Terms of Agreement” document is being prepared, to be signed by ABIVIDRO, the Centro Paula Souza and representatives from CeRTEV. This document will list the curricula and a technical summary of the course contents. We expect the first course to be offered in the first semester of 2015.

Group B: Diffusion of basic and glass science

ACIEPE

During the past two semesters, CeRTEV planned and offered an UFSCar/ACIEPE (Atividades Curriculares de Integração de Ensino, Pesquisa e Extensão, - activities for the integration of education, research and extension) event spearheaded by the UFSCar's Rectorate. In this activity, undergraduate students from UFSCar, under the supervision of a CeRTEV member and UFSCar faculty, have access to a public elementary school, in which they present and discuss some topic in basic science. In a second step, those elementary school students, aged 9-12 years, visit the Laboratório de Materiais Vítreos, LaMaV/DEMa/UFSCar, one of the main CeRTEV's

laboratories. CeRTEV's ACIEPE is entitled "Engineers and Scientists of the Future". Its main objective is to inspire in children younger than 14 years an interest in the physical sciences. We want to eradicate in these children, many of whom come from economically underprivileged backgrounds, the notion that science is "too difficult" or "it is not for me". We demonstrate to them, with simple experiments and demonstrations (e.g. glass melting) what is science and what is the "scientific method". This activity involves about 30 graduate students and 200 elementary school students per year, and has been most satisfactory for all participants.

Other activities

Lectures in elementary public schools.

The Municipality of São Carlos organizes a program called "Science at School", in which the Municipality wants to build a list of lectures to be offered to public elementary and high schools. Upon request of the Municipality, we prepared a list of 14 basic science lectures, to be offered by CeRTEV members, but also other faculty from the Materials Engineering Department at UFSCar. Topics include: *The career of a Material's engineer; How does science work?; Glass crystallization for the fabrication of new materials; Glass and its applications in modern society; Glass production and recycling; Biomaterials: the future of medicine; Optical glasses; Electronic Microscopy: from objects to atoms; From atoms to materials; Materials Science as a base for engineering.*

"Comics"

To illustrate the lecture "Glass and its applications in modern society" we are preparing a "Mangá" - Japanese style "comics" - to introduce some aspects of glass material or the question "what is a glass" to students in elementary school. We plan to prepare such "comics" for all proposed lectures.

"Science on stage"

In association with the group "Ouroboros" for scientific dissemination, we are organizing the event "**Science on stage VIII: science and art meeting**", to be held in São Carlos from August 6th to 10th, 2014. This event will bring together thirteen groups, from Brazil and Portugal, specialized in the arts of dissemination of science through theater. It is expected that, during the four days of this event, one hundred attendees will go through the planned workshops ("*oficinas*") and one thousand people will attend the shows.

Congress Participation

One CeRTEV associate participated in the "13th International Public Communication of Science and Technology" held from May 5th to 8th in Salvador, Bahia. This year, the main theme of the congress was "Science Dissemination for Social Inclusion and Political Engagement". Our associate contributed with two abstracts: http://www.pcst-2014.org/images/abstract_13thpcst.pdf: abstract 20552 - Magic X Science: Ouroboros Science Theater, and abstract 20678 - Sigma PI: Comics and Science Communication.

The attendees presented research work results, performances, workshops, panels and debates related to different issues and points of views. Research results and initiatives to promote access to education and science goods to low income people; access to science spaces and science goods to people living in remote areas; the language and cultural context understanding of immigrants who have difficulties; science communication activities in general. All the participants were very engaged in these purposes, helping the achievement of the event goals, evoking the debate on how to raise more inclusive strategies, both in developing, emerging countries and the developed world, as well as to improve citizenship through public engagement in science and technology and building novel models and practices for communication and participation. This congress alerted us to some specific issues related to the Communication of Science in its entire breadth and relevance. Specially, the theme of "Social Inclusion" is a very important subject in the Brazilian reality.

General activities

We participated to the "Encontro de Coordenadores de Educação e Difusão" 1st Meeting of CEPIDs Education and Outreach Coordinators" held at Ribeirão Preto, 24th and 25th of May, 2014. During this meeting,

Coordinators of Education and Outreach of 15 FAPESP CEPIDs had the opportunity to present their project and to familiarize themselves with projects and experiences from others.

During this meeting, some joint activities between all CEPIDs were planned: i) to make joint expositions about basic science, for instance in the gardens of “Instituto Butantã” in São Paulo (an institution involved in one of the CEPIDs), which receives thousands of visitors per week, especially during weekends. Also, those CEPIDs who already make expositions, for instance, in the “Metro” of São Paulo city, have declared their willingness to include other CEPIDs as a part of future joint endeavors. We are planning a web-site where education activities of all CEPIDs are listed.

Finally, during the 1st Joint Meeting of German Society of Glass Technology (DGG) – and the Annual Meeting of Glass & Optical Materials Division of the American Ceramic Society (ACerS GOMD), which took place in Aachen, Germany, May 25 – 30, 2014, there was a meeting of the Technical Committee 23 – “Glass Education” (TC 23) of the International Commission on Glass (ICG). The Brazilian representative to the TC23 (Ana Rodrigues) is a CeRTEV member, and participated in this meeting. It was proposed to organize a Winter School of Glass, following the concept of the traditional “Montpellier Summer School”. This “Glass Science School” planned by CeRTEV will be incorporated into the overall ICG agenda.

The CeRTEV team considers the organization of scientific, technological and education related congresses a key activity for discussion and disseminations of science. In this first year we were quite active in this area and organized the following congresses:

ACIESP - Os Desafios da Invenção e Inovação no Brasil: Experiências de Sucesso e Insucesso no Estado de São Paulo. São Carlos – SP, 20 de setembro de 2013. <http://agencia.fapesp.br/17814>

1º Workshop - Rede de Biomateriais LaMaV – BIONETEC.

São Carlos – SP, 22 e 23 de novembro de 2013. <https://bionetec2013.oevento.com/>

Internal Workshop CeRTEV 2013 – São Carlos – SP, 08 de outubro de 2013.

<http://www.certeve.ufscar.br/documentos/arquivos/workshop-certeve-programacao>

Humboldt Kolleg - Ciências e Tecnologia na Vida Contemporânea: Impactos e horizontes –

Campos do Jordão - SP, 28 a 30 de September de

2013. <http://www.sbpomat.org.br/12encontro/symposia/humboldt.php>

SBPMat 2013 - Symposium A – Sol-Gel Materials: From Fundamentals to Advanced

Applications. Campos do Jordão - SP, 30 de September. - 02 outubro 2013.

http://sbpmat.org.br/12encontro/symposia/a_symposium.php?lang=en

Workshop sobre Sol-Gel / Química e Processos para a Cerâmica, Compostos e Materiais Híbridos

Inorgânicos-Orgânicos. São Carlos - SP, 04 a 06 de outubro 2013. <http://sol-gel.iqsc.usp.br/>

TECHNOLOGY DEVELOPMENT and TRANSFER

Overview

The research insights obtained from the CeRTEV activities is channeled for generation of new technologies and patents, all the way to new products and production processes (“science to business approach”). As discussed in the research plan and in the scientific section of this report, promising new technologies are expected in five main fields of application: 1) strong GCs for armors and dental implants, 2) bioactive materials for bone and tissue restoration, 3) energy storage and conversion systems, 4) photonic devices, and 5) catalysts for converting biomass into fuels and chemicals. In all these fields we will vigorously pursue transferring fundamental and applied research activities to the productive sector.

We aim at developing of new or improved, patentable glass or glass-ceramic materials in each field of application above: 1) light armors (for use in airplanes, cars and individuals) and tougher monolithic glass-ceramics for dental restoration. In this application field we are working closely with some companies, such as Vitrovita and Cellmat; 2) macroporous and hierarchically ordered scaffolds, fibers, small monolithic parts and powders with increased osteoinductive activities, combined with the ability for targeted drug delivery for bone and tissue repair. Our industrial collaboration network in this area also includes Vitrovita, DMC and Vetra; 3) fast-conducting solid electrolytes for lithium ion batteries. Lithium ion cells in which these electrolytes are being implemented will be developed in São Carlos and tested in collaboration with the Münster Electrochemical Energy Technology center in Germany, a joint academic and industrial platform dedicated to the development of high-energy and high-power lithium ion batteries. We also aim at designing new glass-ceramic seals for fuel cell applications. The Brazilian giants Petrobras and Itaipuare interested in these materials; 4) solid state lasing materials with enhanced emission characteristics. In this area we are still searching for suitable industrial partners. 5) we intend to use our conceptual understanding and research expertise in ceramic design for developing an entirely novel application of glass-ceramics: the conversion of biomass into fuel and fine chemicals. The properties and performance of these catalysts will be tested in collaboration with colleagues at the Brazilian Laboratory of Bioethanol Science and Technology (CTBE) and the Brazilian Laboratory of Synchrotron Light(LNLS). Other industrial collaboration partners will be approached in concert with the research advances made in each area.

The strategy for innovation and technology transfer of our CEPID is based on and follows three basic concepts and actions: *i)Establishment of cooperation agreements and licensing of on-demand technologies commissioned by industry*; the widespread skills of the group will be focused in order to put industries in contact with the three academic institutions; cooperation programs connecting universities, companies and other institutions (PITE and PPP/FAPESP, and FINEP) will be strongly encouraged; *ii)Nucleation of spin-off companies from the group activities*; funds will be sought through programs such as PIPE/FAPESP; and *iii)Extensive promotion of innovation and technology transfer*; accomplished by our extensive know-how in these matters combined with the assistance of agencies at UFSCar (www.inovacao.ufscar.br) and USP (www.inovacao.usp.br).

In collaboration with our partners from industry the technological core of our group is also in the process of establishing infrastructure for the production of prototypes, on a scale beyond the laboratory, bringing our activities closest to the productive sector, e.g., one melting furnace for larger glass volumes than the conventional lab scale (several kilograms instead of grams); one disc mill that can be continuously operated, for a high output of glass powders; and a lab spray dryer for conditioning powders into granules with suitable properties for a fine ceramic processing.

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

In this first year of CeRTEV, several actions were taken to establish cooperation agreements and licensing of technologies commissioned by industry or being developed by the CeRTEV team and which are of interest for commercial production. E.D. Zanotto (CeRTEV Coordinator) has established Non-Disclosure Agreements (NDA) with the following glass companies or companies with glass-based products, whose importance is measured worldwide: Ivoclar Vivadent (Liechtenstein), AGY (EUA), Owens-Illinois (USA), and DMC (Brazil). H. Eckert (CeRTEV Vice-Coordinator) has also established Non-Disclosure Agreements with top glass companies: Nippon Electric Glass (NEG) and Ivoclar Vivadent.

E.D. Zanotto has been consulted on the choice of São Carlos for installation of a plant manufacturing the traditional artistic glass from Murano, Italy. The company considers installing a Murano glass factory, the first one abroad, in the State of São Paulo. For establishing this site, São Carlos is considered a strong contender, owing to the presence of CeRTEV and the strong academic and research programs at UFSCar and USP in the area of glass science.

Contracts for technology development were signed between the CeRTEV team at UFSCar and the Aerospace Technical Center (CTA), a division of Brazilian Aeronautics, aiming at developing of glass-ceramic armors.

At EESC/USP, Raúl Revelo Tobar, a master student under supervision of E.B. Ferreira, has developed a research project for recycling the glass of CRT monitors into glazes for tiles. This effort is an important step in establishing a relationship with the ceramic tile industrial pool of Santa Gertrudes, SP, at ~70 km of São Carlos,

one of the largest in the world. A formalized partnership is currently being established with the Ceramic Center of Brazil (CCB), a private institute with facilities for characterization and certification of ceramic tiles under standard practices, and close relationship with several companies.

Extensive promotion of innovation and technology transfer

CeRTEV Meeting in the 5th Week USP on Intellectual Property and Innovation.

On August 13, 2013 a team of CeRTEV researchers attended a meeting with Eduardo Brito, Administrative Analyst, and Freid Artur, Innovation Agent of the USP Agency for Innovation, during the 5th Week USP on Intellectual Property and Innovation. At this occasion, the following seminars were presented by E. Brito: (i) Legal Framework, Regulatory Frame work and Incentives for Innovation; and (ii) University/Industry Partnership– Formalization, Benefits, Rights and Duties. The oral presentation was accompanied by questions and answers on the specific demands of the CeRTEV members.

Lecture:"The Brazilian Glass Industry and the Potential of Relationship with Universities"

On August, 30, 2013, as an action of the CeRTEV Tech-Transfer Coordination, Dr. Mauro Akerman presented at EESC/USP the lecture "*The Brazilian Glass Industry and the Potential of Relationship with Universities*", targeting the CeRTEV team and the general public. Dr. Mauro Akerman has 30 years of industrial experience at Saint Gobain Glass in Brazil as an internal consultant in the area of glass processing and management of technical training programs. He has retired in 2008 and has since served as an independent consultant in the area. Besides, he is the coordinator of the School of Glass associated with ABIVIDRO (Brazilian Technical Association of Automatic Glass Industries) and coordinator of the technical committee of ABIVIDRO. He presented a panel on the Brazilian glass industry, ongoing developments, building of new furnaces, e.g., for flat glass and packaging, as well as new processing plants, the challenge of specialized technical training for glassmaking, and areas of potential collaboration between universities, research centers and the glass industry.

Symposium on Innovation in São Carlos and São Paulo

On September 20, 2013, the Symposium "*The challenges of invention and innovation in Brazil: experiences of success and failure in the State of São Paulo*", was held at UFSCar, São Carlos. This meeting was sponsored by the Academy of Sciences of the State of Sao Paulo (ACIESP) and organized by E.D. Zanotto, member of the ACIESP and Coordinator of CeRTEV. The invited speakers are recognized authorities with extensive experience in product development, processes, patents, interactions with companies, research and management of science and technology. The Symposium discussed the process of invention and innovation in universities and companies, and especially the experiences conducted in the State of São Paulo. The event was open to students, teachers, researchers, entrepreneurs, journalists and the interested public. About 100people attended the symposium. The event was covered by the press, e.g.: <http://agencia.fapesp.br/17876>, and <http://www.dci.com.br/sao-paulo/simposio-em-sao-carlos-discute-inovacao-id364282.html>. Please find attached the Symposium poster.

Patents filed

The following patents were filed in the Brazilian National Institute of Industrial Property (INPI) by some of CeRTEV researchers, as solid results of their scientific and technological efforts in the main fields of interest of our CEPID.

BR 10 2013 017769 5 "Glass-ceramic compositions, obtained glass-ceramic from the same, armor of sacrifice, and ballistic protection armor" (in Portuguese); Titular: UFSCar; Inventors: Leonardo Sant'Ana Gallo, Ana Cândida Martins Rodrigues, **Oscar Peitl Filho**, **Edgar Dutra Zanotto**; deposited in June 26, 2013.

BR 10 2013 020961 9 "Glass composition, fiber and bioactive vitreous fabrics obtained from the same, and articles obtained by the same" (in Portuguese); Titular: UFSCar; Inventors: **Edgar Dutra Zanotto**, Marina Trevelin Souza, **Oscar Peitl Filho**; deposited in August 12, 2013.

BR 10 2014 003817 5 “Discontinuous coating process using a bio absorbable and bioactive biomaterial applied to solid substrates, the discontinuous coating obtained by same and the use of the discontinuous coating obtained by same” (in Portuguese); Titular: UFSCar; Inventors: **Edgar Dutra Zanotto**, Clever Ricardo Chinaglia, **Oscar Peitl Filho**; deposited in February 19, 2014.

These patents are being analyzed at INPI, which may take from 7 to 10 years. They are also being analyzed by the UFSCar Innovation Agency for a Patent Cooperation Treaty (PCT) application.

The internet discussion list denominated "vidros"

The discussion list in the Internet denominated *Vidros*, created in 1997 by the Coordinator of Tech Transfer E.B. Ferreira, formerly in the address vidros@listas.ufscar.br and hosted at the UFSCar General Secretariat for Information (Sin), was brought to a more modern and attractive virtual environment: *lista vidros* at <https://groups.google.com>, whose e-mail is now listavidros@googlegroups.com. The member list increased from about 100 to 160 participants in academy and industry, and still has a large growth potential. Active people in the glass field have been invited to join and participate, stimulating the relationship and R&D activities between academy and industry.

Peão da Tecnologia

E.D. Zanotto received at the end of April 2014 the award "Pawn of Technology". Created by the Technological Park Foundation of São Carlos (Parq Tec) in 1993, the titles awarded to people who have contributed, through technological innovation, to increase production, quality and competitiveness of products, processes and services in companies. The award was widely covered by the press, e.g.: <http://agencia.fapesp.br/19052>, <http://sbpmat.org.br/professor-edgar-zanotto-recebe-o-titulo-de-peao-da-tecnologia-por-suas-aco-es-em-prol-do-desenvolvimento-de-sao-carlos/>, http://www.abc.org.br/article.php3?id_article=3330, <http://sinc.com.br/pesquisadores-de-sao-carlos-sp-recebem-titulo-de-peao-da-tecnologia.html>, <http://www.abividro.org.br/noticias/edgar-dutra-zanotto-recebe-o-titulo-de-peao-da-tecnologia>, etc.



"Os desafios da invenção e inovação no Brasil: Experiências de sucesso e insucesso no Estado de São Paulo"

São Carlos
Dia 20/09/2013
Auditório Bento Prado Jr.
da UFSCar

8:30h Abertura
Targino de Araújo Filho - Reitor da UFSCar
José Eduardo Krieger - Presidente da ACIESP
Edgar Dutra Zanotto - Conselheiro da ACIESP

Experiências em São Carlos

- 9:00 - **Sérgio Mascarenhas** - Coordenador de projetos do Instituto de Estudos Avançados IEA-USP São Carlos
- 9:20 - **José Galizia Tundisi** - Secretário de C & T de São Carlos, Presidente do CNPq (1995-1999)
- 9:40 - **Milton Ferreira de Souza** - Fundador do Parqtec São Carlos, criador de 5 empresas
- 10:00 - **Vanderlei Salvador Bagnato** - Coordenador do CEPID CEPOF e da Agência USP de Inovação
- 10:20 - **Elson Longo** - Professor Titular do IQ-UNESP Araraquara, Coordenador do CEPID CMDMC da UFSCar
- 10:40 - **Oswaldo Novais de Oliveira Jr.** - Professor Titular do IFSC, Coordenador de uma rede de Nanobiotecnologia
- 11:00 - **Edson Roberto Leite** - Professor Titular do DQ-UFSCar
- 11:20 - **Mariana A. Lima Braulio** - Doutora em Engenharia de Materiais Engenheira de Pesquisa, Desenvolvimento e Inovação da ALCOA

Experiências no Estado de São Paulo

- 14:00 - **José Arana Varela** - Diretor Presidente da FAPESP, Professor Titular do IQ-UNESP
- 14:30 - **José Fernando Perez** - CEO da Recepta BioPharma, Diretor Científico da FAPESP (1993-2005)
- 15:00 - **Fernando Reinach** - Gestor do Fundo Pitanga de Investimento, Ex-secretário de desenvolvimento científico do Ministério de Ciência e Tecnologia
- 15:30 - **Sérgio R. R. de Queiroz** - Coordenador Adjunto de Pesquisa para Inovação da FAPESP, Professor Associado do DPCT/IG/UNICAMP
- 16:00 - **Vanderlan Bolzani** - Diretora da Agência UNESP de Inovação Professora Titular do Instituto de Química
- 16:30 - **José Eduardo Krieger**
Edgar Dutra Zanotto **Encerramento**

Os palestrantes são autoridades reconhecidas e têm extensa experiência no desenvolvimento de produtos, processos, patentes, interação com empresas, estudos e administração de ciência e tecnologia. Esta reunião tratará o processo de invenção e inovação nas universidades e empresas e especialmente estudos realizados no Estado de São Paulo. Será aberta a estudantes, professores, pesquisadores, empresários, jornalistas e ao público interessado.

Inscrições:

Enviar email para: aciesp@acadciencias.org.br

Colocar no assunto da mensagem:

"Simpósio Inovação São Carlos" e no

corpo da mensagem: Nome, endereço e cargo atual

Edgar Dutra Zanotto
Conselheiro da ACIESP
Professor de Engenharia de Materiais
LaMaV - Laboratório de Materiais Vitreos
Departamento de Engenharia de Materiais
Universidade Federal de São Carlos
<http://lamav.weebly.com>
<http://www.certev.ufscar.br>

José Eduardo Krieger
Presidente da ACIESP
Professor de Genética e Medicina Molecular
Escola de Medicina
Instituto do Coração
Universidade de São Paulo
krieger@incor.usp.br



5. Institutional support (2 pgs).

The CeRTEV has 7 faculty from UFSCar (including the center manager), 6 from USP- São Carlos campus, and 1 from UNESP - Araraquara campus.

Institutional commitment UFSCar

The institutional support offered by UFSCar to our center has been quite substantial and helpful.

A young faculty (Dr. Marcello R. B. Andreetta) was hired by the Department of Materials Engineering - DEMa - and immediately joined the CeRTEV team.

A new secretary, with a degree in administration (miss Ligia Diniz) was also hired for by Vitreous Materials Lab of DEMa (CeRTEV's headquarters). She has been of tremendous help with all the administration of 15 faculty and about 50 students of the center.

Additionally, an intern in computer science (Mr. Henrique Guarnieri), was also hired and spends 12 hours per week at LaMaV giving support to all computer maintenance and construction of the webpage (www.certeve.ufscar.br)

Finally UFSCar research administration office head (Ms. Bruna Moraes) has also been of great help with all the complex materials purchasing bureaucracy and especially importation of materials and equipment of the CeRTEV team.

UFSCar's audio and teleconference facilities have also been offered to us and will be used starting next year.

Institutional commitment USP

Besides the USP institutional commitment already very much detailed in the CEPID first proposal, below we point the extra support which arose in respect of CeRTEV activities, or that guarantee to a large extent its activities.

Physical space

In January, 2014, the Group of Ceramics of the Department of Materials Engineering (SMM), EESC, moved from a lab of 40m² in the former SMM building at USP's Area 1 in São Carlos, shared with three principal investigators, to completely new facilities in the campus Area 2. The new ceramic lab now has 291m². The new SMM totals approximately 4,500m², which includes the investigators' office and several labs of general purposes (user facilities): thermal analysis, chemistry lab, machine shop, thermal treatments, mechanical property characterization, sample preparation, optical and electrical microscopy, and x-ray diffraction, among others, besides the ceramic-specific labs. About US\$ 3,120,000.00 has been spent in building, facilities and purchasing equipment, materials and costs, funded by University of São Paulo.

IFSC made 50m² of space available to house the new NMR spectrometer acquired by CeRTEV. Regarding the ESR lab, it had significant improvements done when the EPR machine was moved to its space. USP has provided funds for purchase of construction materials, electrical installation, internet network, materials and labor for building and facilities.

Research support at IFSC and EESC-USP

The Hybrid Materials Technology Center (CTMH/USP) is an interdisciplinary and multidisciplinary partnership for research, development and innovation in hybrid materials and materials interrelationships during fabrication processes, which joins the SMM/EESC with the Group of Crystal Growth and Ceramic Materials of the Physics Institute of São Carlos (IFSC). The CTMH started its activities in 2011 with an initial budget of US\$ 500,000 for a Scanning Electron Microscope with Field Emission Gun (SEM/FEG) and EDS, and US\$ 17,000.00 for materials and costs, funded by USP. These facilities are already available at EESC and

running quite properly. USP is also responsible for the salary of the specialized technician responsible for operating the equipment.

Innovation support at EESC and IFSC-USP

The USP Agency for Innovation assisted us during the *CeRTEV Meeting in the 5th Week USP on Intellectual Property and Innovation*, detailed in the Tech Transfer Section of this Report. It also gave us support on the analysis of a research contract being formalized between the Itaipu Technological Park and EESC.

Institutional commitment of UNESP

The Chemistry Institute of UNESP in Araraquara has provided all the means necessary for the development of this project. Just after Prof. Marcelo Nalin's hiring and arrival in Araraquara (May 2013), the head of the Inorganic Chemistry Department and Dr. Sidney Ribeiro offered space in his laboratory to arrange all the equipment and to accommodate Dr. Nalin's students. This laboratory, now shared with Prof. Ribeiro's group, has around 200m² with numerous facilities. Small adaptations of the local infrastructure were necessary concerning air conditioning, electricity panel, etc. to accommodate the equipment. The institute director also assumed the responsibility and of feredall the necessary furniture for Dr.Nalin's laboratory. In the Institute they have some multi-user equipment, to which the Nalin group has total access. Therefore the support given to Nalin and his group was quite substantial.

6. Plans for next year (max 2 pgs).

FUNDAMENTAL RESEARCH - Plan of New Activities for Year 2

A top priority for CeRTEV's success will be the development of a coherent research programme aligning the activities of its individual members towards the common CeRTEV objectives. Towards this purpose about 10 planning meetings have taken place during the past year, and joint activities have already begun. In the area of *armor and dental ceramics*, the possibility of monitoring nucleation and crystalline via ⁷Li-²⁹Si cross-polarization NMR will be built upon in an effort to study the nucleation process in its early stages. Our preliminary results indicate that NMR spectroscopy can be used in-situ for monitoring nucleation by direct observation. Another promising technique to be explored in detail is Raman spectroscopy, which will be conducted in parallel with the NMR studies done in an effort to relate the spectroscopic observables of both methods. Armed with these two powerful techniques and their potential synergy we expect to address some long-standing fundamental questions regarding the validity of the classical nucleation theory. In addition, we have begun exploring the dynamics of lithium disilicate melts by molecular dynamics simulations. These studies will be extended to reach a deeper understanding of the nucleation kinetics in these systems. We will further extend these studies to lithium diborate glass, another material well known to undergo volume (as opposed to surface) crystallization. In the area of *bioglasses* fundamental questions regarding the structural role of magnesium oxide (network former versus network modifier) will be addressed, applying vibrational spectroscopy and NMR *in tandem* to some new promising magnesium borate containing compositions. With the imminent arrival of the new 600 MHz solid state NMR spectrometer we will be able to develop the potential of the low-gamma quadrupolar nucleus ²⁵Mg for probing the structural environment of magnesium ions in glasses in a direct fashion. Work in the *modern energy technology area* will focus on correlating electrical conductivity measurements with dynamic observables (two- and three-time correlation functions) extracted from sophisticated multidimensional NMR experiments in the lithium-based NASICON ceramic system. In addition we will gradually shift our focus upon including sodium-containing materials into our research agenda, as these materials offer much higher sustainability than lithium-based solid electrolytes. Contrary to the situation with ⁷Li NMR, the ²³Na nucleus is affected by much stronger quadrupolar interactions, which demand a significant alteration in the spectroscopic strategy for dynamical characterization. Accomplishing this objective will require a major effort, both on the experimental and the computational side. In the area of *photonic materials*, we will build upon the very promising results obtained within the first year regarding the development of (a) new fluorophosphate glass and glass-ceramic compositions as solid hosts for rare-earth ion emitting laser materials, and (b) glasses containing uniformly-sized metal nanoparticle emitters. Glasses with optimized photophysical properties will be selected for detailed ceramization studies, which will be followed by NMR, EPR, and Raman spectroscopies. Finally, in the area of *catalytic materials* we will commence with the elaboration of solution templating preparation methods for the generation of hierarchically structured materials, containing both meso-

and macropores. The materials produced in this fashion will then be surface functionalized with layers of suitable transition metal oxide species (titania, niobia, vanadia, molybdenum oxide etc.), characterized structurally and subjected to suitable catalytic test reactions. As such hierarchically structured materials are also very promising for osteoprotective and –inductive applications, we will also test them with respect to their interaction with simulated body fluid and osteoblastic cell cultures.

In summary, by the end of year 2 we expect to have developed the full range of activities in all of the areas delineated in the original CeRTEV proposal, and we anticipate to reap the first synergetic benefits obtained from results in the different application fields. We anticipate that as the result of our research efforts we will by then have various excellent glassy and glass-ceramic systems available whose technological application (and commercialization) potential can be studied further together with our partners in industry.

EDUCATION and OUTREACH- Plan of New Activities for Year 2:

Next semester, we will continue our efforts to make the Glass Technical Course (Centro Paula Souza/ABIVIDRO) a reality for the first semester 2015.

Our ACIEPE activities will be continued on a regular basis. All materials used in this ACIEPE are being improved. We will also evaluate the impact of these activities on the participating children, by means of short questionnaires to be answered before and after the events.

We are also planning to organize educational kits with colored glasses. An optical kit for demonstration of optical phenomena for undergraduate or high school students is already available. We are planning to make use of these kits within the program “Science in School”, from São Carlos Municipality. Finally, we will start collecting exhibits for our planned glass museum.

TECHNOLOGY DEVELOPMENT AND TRANSFER -Plan of New Activities for Year 2

Our strategy for technology transfer and innovation was detailed in the CEPID proposal. We will mostly continue on the path traced there, in CEPID’s 2nd year. In summary, it is based on the concepts and actions detailed below:

Establishment of cooperation agreements and licensing of on-demand technologies commissioned by industry:

Several agreements between the CeRTEV team and companies interested in glass and glass-ceramic technologies have already been formalized, as stated in the Tech Transfer Section of this report. Others are currently being negotiated or on the way to be formalized. For the second year, we plan to consolidate the transfer of technologies based on scientific and technological researches accomplished by our team, together with the partnership with these companies. The corresponding results will be documented in the form of new prototypes and filed patents. Technology licensing will be always pursued as a result from the agreements mentioned above.

Nucleation of spin-off companies from the group activities:

This is, of course, the most challenging project. But we already have confidence and indications that the first results can be presented soon.

Promotion of innovation and technology transfer:

We will continue our efforts to establish facilities for the production of prototypes, on a scale beyond the laboratory. As planned, one melting furnace for larger glass volumes than the conventional lab scale and one disc mill, which can be continuously operated for relatively large production of glass powders, have already been acquired at EESC/USP and will be installed and start operating in this 2nd year. A lab spray dryer for

conditioning powders into granules with suitable properties for fine ceramic processing is currently being acquired.

In a partnership with the UFSCar and USP Agencies for innovation, we will organize a workshop to stress to the group members and collaborators how to detect interests and manage some of their research to innovation, to follow the patent literature, to get access to patents and market reports, to estimate production costs and the potential market for a given technology, to avoid publications prior to patent request, and other important issues.

The discussion list in the Internet denominated *Vidros*, brought in the 1st CeRTEV year to a more modern and attractive virtual environment: *lista vidros* at <https://groups.google.com> and listavidros@googlegroups.com, will be in focus aiming to increase the number of participants interested in glasses and glass-ceramics, in academy and industry. We will start a campaign to invite active people in the glass field to join and participate, stimulating the relationship and R&D activities between them.

It is a common sense there is a big gap between industry and academy in the field of glasses in Brazil, as in many other technologies. The largest companies installed in the country are mostly multinational with their head quarters and R&D labs abroad. The activities in this country are mainly focused on production and commercialization, attracted by a colossal internal market and on relative low costs of raw materials, manpower and production, and much less on development of new technologies and IP, from which the economical benefits would increase exponentially. We can observe such a big mismatch between academy and industry even for companies with domestic capital, which look abroad for the technologies they demand, transferring to foreign countries the impact of their economical activities. This is true to an even larger extent in the field of glass-ceramics, a high-tech material. After many years of experience on higher education of our CeRTEV team, we have clearly identified the current deficits of affordable technical information in the field as one of the main barriers to break this vicious cycle of underdevelopment, which translates to a large extent in lack of specialized literature in Portuguese. From this awareness, for the CeRTEV 2nd year, we plan to start writing and make accessible in Portuguese a book on Glass Technology, having the workers in industry and students in the field as the main target public. We have already identified several specialists on aspects of the glass production in Brazil, with solid experiences in the glass industry, willing to collaborate in this challenge. For this, we rely on the important partnership with Dr. Mauro Akerman, who has 30 years of industrial experience at Saint Gobain Glass in Brazil as an internal consultant in the area of glass processing and management of technical training programs, now retired. Since 2008 Dr. Akerman has served as an independent consultant in the area; besides, he is coordinator of the School of Glass associated with ABIVDRO; and coordinator of the technical committee of ABIVIDRO. By the time of the next report, we intend to have this book already in an advanced state of writing.

8. List of publications resulting from the grant to which the report refers Scientific (including accepted for publication, stating in each case this situation) in the period, grouped in the following categories:

- **Congresses organizad by the CeRTEV members in this period**

ACIESP - Os Desafios da Invenção e Inovação no Brasil: Experiências de Sucesso e insucesso nenhum Estado de São Paulo. São Carlos – SP, 20 de setembro de 2013.

<http://agencia.fapesp.br/17814>

1º Workshop - Rede de Biomateriais LaMaV – BIONETEC. São Carlos – SP, 22 e 23 de novembro de 2013.

<https://bionetec2013.oevento.com/>

Workshop CeRTEV 2013 – São Carlos – SP, 08 de outubro de 2013.

<http://www.certev.ufscar.br/documentos/arquivos/workshop-certev-programacao>

Humboldt Kolleg - Ciências e Tecnologia na Vida Contemporânea: Impactos e horizontes – Campos do Jordão - SP, 28 a 30 de September de 2013.

<http://www.sbpmat.org.br/12encontro/symposia/humboldt.php>

SBPMat 2013 - Symposium A – Sol-Gel Materials: From Fundamentals to Advanced Applications. Campos do Jordão - SP, 30 de September. - 02 outubro 2013.

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Workshop sobre Sol-Gel Química e Processos para a cerâmica, composto e Materiais Híbridos Inorgânicos-Orgânicos. São Carlos - SP, 04 a 06 de outubro 2013.

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a. Articles in scientific journals;

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FRAYGOLA, B.; MESQUITA, A.; COELHO, A.A.; GARCIA, D.; MASTELARO, V.R.; EIRAS, J.A. **Fe valence fluctuations and magnetoelastic coupling in Pb-based multiferroics perovskites.** *Physica Status Solidi (A) Applications and Materials Science*, V. 210, Issue 2, Pages 386-390, 2013.
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OLIVEIRA, L.H.A., PARIS, E.C.B., AVANSI, W.C., RAMIREZ, M.A.D., MASTELARO, V.R.E., LONGO, E.C., VARELA, J.A. **Correlation between photoluminescence and structural defects in Ca_{1+x}Cu_{3-x}Ti₄O₁₂ systems.** *Journal of the American Ceramic Society*, V. 96, Issue 1, P. 209-217, 2013.

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- **List of publications resulting from the grant to which the report refers Scientific - accepted for publication.**

RINO, J. P.; *An interaction potential for barium sulfide: A molecular dynamics study.*

Trabalho aceito no Computational Materials Simulation

Trabalho aceito para publicação no Computational Materials Science

GABBAI-ARMELIN, P. R.; Souza, M. T.; Kido, H. W.; Tim, C. R.; Bossini, P. S.; MAGRI, A. M. P.; FERNANDES, K. R.; MAGRI, A. M. P.; PARIZOTTO, N. A.; FERNANDES, K. R.; MESQUISTA-FERRARI, R. A.; RIBEIRO, D. A.; PEITL-FILHO, O.; RENNO, A. C. M. *Characterization and biocompatibility of a fibrous glassy scaffold.*

Trabalho submetido a Journal of Tissue Engineering and Regenerative Medicine

GABBAI-ARMELIN, P. R.; SOUZA, M. T.; KIDO, H. W.; TIM, C. R.; BOSSINI, P. S.; MAGRI, A. M. P.; FERNANDES, K. R.; PASTOR, F. A. C.; ZANOTTO, E. D.; PARIZOTTO, N. A.; PEITL-FILHO, O.; RENNO, A. C. M. *Effect of a new bioactive fibrous glassy scaffold on bone repair.*

Trabalho submetido a Journal of Materials Science: Materials in Medicine

CARDOSO, D. A.; GABBAI-ARMELIN, P. R.; ZANOTTOD, E. D.; PEITL, O.; LEEUWENBURGH, S. C. G.; JANSEN, J. A.; RENNO, A. C.M.; BEUCKEN, J. J. J. P. VAN DEN. *Injectable composites based on biosilicate® and alginate: handling and in vitro characterization*

Trabalho em fase de reajustes e submissão)

BESSE, V.; FORTIN, A.; BOUDEBS, G.; VALLE, P.S.; NALIN, M.; DE ARAUJO, C.B. “*Picosecond nonlinearity of GeO₂-Bi₂O₃-PbO-TiO₂ glasses at 532nm and 1064 nm Applied.*”

Trabalho submetido Physics B: Laser and Optics

b. Articles in non-indexed journals;

c. Papers presented at international conferences;

“TAB meeting / Owens-Illinois, Perrysburg, USA 09 a 12/03/2014”

ZANOTTO, E. D.. *CeRTEV A new glass research center in Brazil-* (Invited)

“Glassman, SP 13/03/2014”

ZANOTTO, E. D.. *CeRTEV- A new glass research center in Brazil-* (Invited)

“AADR/CADR Annual Meeting & Exhibition, Charllote, N.C. - 2014”

CHINELATTI, M.A.; TIRAPELLI, C.; CORONA, S.A.M.; ZANOTTO, E.D.; PEITL-FILHO, O.; PANZERI, H. *Effect of Biosilicate® on Dental Erosion.*

“Glass Research Summit / Corning Incorporated. USA 10 a 15 Jun 2014”

ZANOTTO, E. D.. *40-years of crystal nucleation in glasses.* (Invited)

**“Workshop on “Photoluminescence in Rare Earths: Photonic Materials and Devices (PRE’14),
realizado de 13 a 16 de maio de 2014 em San Sebastian, Espanha”**

MATHIAS, C. F.; MONTESSO, M.; MANZANI, D.; RIBEIRO, S. J.L.; NALIN, M.; “*Optical Studies of Er³⁺/Yb³⁺ Co-Doped Germanium-Antimonate Glasses*” (Oral presentation Marcelo Nalin)

“1st Joint Meeting of DGG-ACerS GOMD Aachen, Germany 25 – 30 May 2014.”

<http://www.dgg-gomd.org/wp-content/uploads/2013/04/DGG-GOMD-2014-Programme.pdf>

JIANG, S.; YOUNGMAN, R.; FELLER, S. A.; ZANOTTO, E.D. *Glass & Optical Materials Division Officers* (Co-organizadores do congresso)

ZANOTTO, E. D.; PEITL, O.; SOUZA, M. T.; CROVACCE, M.; CHINAGLIA, C.; SIQUEIRA, R.; RODRIGUES, A. C. M.; BOCCACCINI, A.; HENCH, L.. *BioSilicate – a multipurpose, highly bioactive glass-ceramic*. (talk by E. D. Zanotto In the congress). Same paper in the Biomaterials Round-Table (invited)

GALLO, L. S.; MOSCA, T. D. M.; TEIDER, B. H.; POLYAKOVA, I. G.; RODRIGUES, A. C. M.; ZANOTTO, E. D.; FOKIN, V. V.; *Effect of Li₂O on the crystallization of Na₂O.2CaO.3SiO₂ glass*. (Talk apresentado por RODRIGUES, A. C. M.)

J. KJELDSSEN, YUE, Y.Z.; RODRIGUES, A.C.M. *Fragility– Structure – Conductivity Relations in Vanadium Tellurite Glass*

CROVACE, M.C.; FORTULAN, C.A.; RODRIGUES, A.C.M.; PEITL, O.; ZANOTTO, E. D. *Macroporous glass-ceramic scaffolds obtained via 3D-printing*

CHINAGLIA, C. R. ; PEITL, O.; SOUZA, C. O. D.; CAMPANINI, L.; MOURA, C. C. G.; BARBOSA, D. Z.; COELHO, P. G.; ZANOTTO, E. D.. *A bioactive glass coating on titanium: A new surface with bactericidal property and enhanced wettability and bioactivity*. (pôster)

SOUZA, M. T. ; RENNO, A. C.; PEITL, O.; ZANOTTO, E. D.. *New highly bioactive glass fibers for skincare*. (apresentado por M. T. Souza)

ECKERT, H. *The mixed network former effect in glasses: structure/property correlations in Phosphate-based glass systems*. (talks presented H. Eckert)

NALIN M.. “*Optical properties of rare earth doped oxide glasses and glass-ceramics containing metallic nanoparticles*”. (Invited talk).

DE CAMARGO, A. S. S. ; GONÇALVES, T. S. ; MOREIRA, R. J. ; ECKERT, H. *Structural-functional correlations in rare earth (RE = Er³⁺, Yb³⁺) doped oxyfluoride glass*. (Poster)

FERREIRA, E.B.; MACENA, G.S.; “*Glass forming ability and microstructure of glass-ceramics in the system Na₂O-CaO-SiO₂*”. (Poster)

FERNANDES, R.G.; FERREIRA, E.B.; “*Calculus of heterogeneous crystallization kinetics of glass particles with regular shapes and comparison with non-isothermal DSC*” (Poster)

RINO, J. P.; GONÇALVES, L. G. *Glass forming ability in Pd₄₅i₅₅ and Pd₃₅Ni₅₅Pt₁₀ mettalic glasses*. (Invited talk)

“Reunião Regional da SBPC no vale do Paraíba – 05 de Junho de 2014.”

Peitl, O e Zanotto. E.D.. *Novos Materiais para a Saúde*. (invited talk)

“13th Lahnwitzseminar on Calorimetry 2014, Rostock, Alemanha, de 15 a 20/06/2014.”

FERNANDES, R.G.; REIS R.M.C.V.; ZANOTTO, E.D.; FERREIRA E.B.; “*The effect of particle size on overall crystallization of diopside glass detected by DSC*”. (poster presentado)

“Rocky Mountain Conference on Analytical Chemistry, Copper, Colorado, USA, July 2014.”

ECKERT, H. *Homonuclear Recoupling Strategies in High Resolution Solid State NMR Spectroscopy: Applications to Inorganic Materials*.

“Academy of Dental Materials Annual Meeting, The Westin Bayshore Vancouver, BC, Canada, Outubro 9 – 12, 2013”

M.D.S. Lanza, M.R.B. Andreeta, R.M. Carvalho, L.F. Pegoraro; “*Degree Of Conversion Of Resin Cements Under A Clinical Simulate Setting*”. Resumo publicado no Dental Materials, 2013; V. 29 (Supplement 1): e44-e45. 2013. (Pôster)

“Conference of Germany, Italy, Slovenia, Frauenchiemsee, Germany, September 2013”

H. ECKERT. *Recoupling of homonuclear dipole-dipole interactions in Multispin Systems: Applications to inorganic materials, Discussion Meeting, GDCh-Magnetic Resonance Section and First Trinational NMR*.

“23rd International Congress on Glass, Prague, República Tcheca - July 7-12, 2013.”

ZANOTTO, E. D. “*Structural similarity/dissimilarity between glass and isochemical crystal and the nucleation ability*”. (invited talk).

GALLO, L.S.A., MEO, C.E., ZANOTTO, E. D., RODRIGUES, A.C.M., *Hard MgO-Al₂O₃-SiO₂ glass-ceramics*. (Pôster).

VILLAS-BOAS, M. O. C.; SOARES, V. O.; ZANOTTO, E. D. “*Analysis of nucleating agents for lithium silicate glass-ceramics*”(Pôster)

SANTOS, G. G.; ZANOTTO, E. D.; FOKIN, V. M. “*Crystallization of CaO-Li₂O-SiO₂ glasses*” (Pôster)

BRAGATTO, C. B., SZEMKUS, S., CASSAR, D.R., RODRIGUES, A. C. M. , *Structural relaxation in AgPO₃ glasses observed through electrical conductivity measurements* (Condução iônica relaxação estrutural vidros fosfato) (Pôster).

MACHADO, M.M., BRAGATTO, C. B., RODRIGUES, A.C.M., *Effect of structural relaxation on electrical conductivity and density and of a soda-lime silicate (window) glass* (Oral).

RODRIGUES, A.M.; MERCURY, J.M.R.; LEAL, V.S., CABRAL, A.A., *Isothermal and non-isothermal crystallization of a fresnoite glass* (Oral).

VALLE, P. S.; NALIN, M. “*Influence of thermal treatment on the optical and structural properties of heavy metal oxide glasses*” (Oral presentation by Marcelo Nalin).

DE CAMARGO, A. S. S. *Optical materials based on Ir(III) complexes incorporated in mesoporous silicate hosts: In situ versus topotactic synthesis approaches and electronic structure analysis*. (Oral)

“24th International Conference of the International Association for the Advancement of High Pressure Science and Technology (AIRAPT) 18th International Conference of the American Physical Society Topical Group on Shock Compression of Condensed Matter (APS-SCCM) Seattle, Washington, from July 7th through July 12th, 2013.”

PIZANI, P.S.; JASINEVICIUS, R.G. " *The effect of high non-hydrostatic pressure on III-V semiconductors: zinc blende to wurtzite structural phase transition and multiphase generation*"

“2013 MRS Spring Meeting & Exhibit, San Francisco, California April 1-5, 2013”

ESCANHOELA, C. A.; BERNARDI, M. I. B.; SILVA, L. F. da; MASTELARO, V.R.. “*Synthesis, characterization and gas sensing properties of $LaxSr1-xTi1-yFeO3$ system*”.
Warrendale: Materials Research Society - MRS, 2013. abstr. S4.108. (Poster)

“2013 MRS Fall Meeting & Exhibit, Boston, Massachusetts - December 1-6, 2013”

MASTELARO, V. R.; AVANSI JUNIOR, W.; RIBEIRO, C.; OLIVEIRA, C. L. P. de; LEITE, E. R. *Morphology evolution of $V2O5/nH2O$ nanostructures in hydrothermal conditions*.
Warrendale: Materials Research Society - MRS, 2013. abstr. R15.47. (Poster)

SCZANCOSKI, J. C.; MASTELARO, V. R.; SIU LI, M.; LONGO, E. L.. *Structural and photoluminescence properties of $SrWO4$ powders synthesized by the co-precipitation and polymeric precursor methods*.

Warrendale: Materials Research Society - MRS, 2013. abstr. R10.22. (Poster)

“6th International Conference on Electroceramics, João Pessoa, Brasil – November 03-13, 2013”

CATTO, A. C.; SILVA, L. F. DA; SCANHOELA JUNIOR, C. A.; AGUIR, K.; MASTELARO, V. R.; LAITHIER, V.. *Co doping effect on the gas sensing properties of ZnO* . (Pôster)

MOURÃO, H. A. DE J. L.; OLIVEIRA, C. R. DE, MASTELARO, V. R.. *Conventional hydrothermal synthesis of pure and Fe-doped $SrTiO3$* . (Pôster)

MASTELARO, V. R.; MESQUITA, A.; BERNARDI, M. I. B.; MICHALOWICZ, A.; EIRAS, J. A.; *Electronic and short-range order structure of $Ba1-yAyTi1-xZrxO3$ (A=La,Ca) : Correlation with normal to relaxor evolution behavior*. (Pôster)

“19th Larson Workshop Indianapolis, IN October 6 – 9, 2013”

ZANOTTO, E. D. “*Crystallization of inorganic glasses: Fundamentals and advanced applications*”. (Invited talk).

“IADR/AADR/CADR General Session and Exhibition, Seattle, WA - 2013”

CHINELATTI, M. A. ; BARBOSA, D. G. P. ; TIRAPELLI, C. ; PIRES-DE-SOUZA, F. C. P. ; PANZERI, H. ; PEITL-FILHO, O. ; ZANOTTO, E. D. . *Adhesion to dentin surface sandblasted with biosilicate microparticles*. USB Abstracts, Journal of Dental Research, v. 92. p. 2790-2790, 2013.

“Annual Meeting of the Brazilian Materials Society, Campos de Jordão, September 2013.”

ECKERT, H. *Modern Solid State NMR Strategies for Studying Structural Transformations in Non-Siliceous Sol-Gel – Glass Systems.*

“Encontro da Associação dos Alunos Alexandre Von Humboldt, Campos de Jordão, September 2013”

ECKERT, H. *Welcome to the Age of Glass.*

“Workshop on Sol-Gel Chemistry, Department of Chemistry, University of Sao Paulo, Sao Carlos, October 2013”

ECKERT, H. *Modern NMR Techniques for the Study of Sol-Gel Glasses.*

“Humboldt Kolleg 2014 – Science and Method – Paradigms and perspectives, Porto Alegre – RS, Abril de 2014.”

Eckert, H. *Spying With Spins on Messy Materials.*

DE CAMARGO, A. S. S. *Fascinating Lasers and their Applications.* (Oral presentation)

“II Seminário Internacional de Cerâmica na Arte-Educação, Cunha, SP, de 24 a 26/10/2013.”

FERREIRA, E.B.; *"Ensino de tecnologia nos cursos de Cerâmica Artística"* (Oral presentation)

“18th International Society of Magnetic Resonance Meeting (ISMAR), Rio de Janeiro, 19 a 24 maio 2013.”

MAGON, C.J.; DONOSO, J.P.; SILVA, I.D.A.; NASCIMENTO, O.R.; LIMA, J.F.; MORENO, M.; BENAVENTE, E.; GONZALEZ, G. *EPR study of copper ethylenediamine intercalated in bentonite clay.* Abstract MO229

MAGON, C.J.; LIMA, J. F.; DONOSO, J. P.; LAVAYEN, V.; BENAVENTE, E.; NAVAS, D.; GONZALES, G. *Deconvolution of the EPR spectra of vanadium oxide nanostructures.* Abstract TU230

APS-SCCN & AIRAPT-24 joint conference, Seattle, USA - July 7-12, 2013.

RINO, J. P.; DASILVA, C.J.: *“Atomistic Mechanism of Plastic Deformation During Nano-indentation in Titanium Aluminide”.* (Oral presentation)

ICMAT2013 - the 7th Biennial International Conference on Materials for Advanced Technologies. Symposium W: Advanced Structural and Functional Materials for Protection, 30 June to 5 July, Singapore, 2013.

RINO, J.P.: *"Atomistic Simulation of Advanced Materials"*. (Invited talk)

“Latin American Osseointegration Congress, São Paulo – SP, 2013.”

CHINAGLIA, C. R.; ZANOTTO, E. D.; PEITL, O.; SANCHES, L.; SOUZA, C.W.O.; CAMPANINI, L. A. *Uma nova superfície de titânio com propriedade bactericida, reduzido angulo de contato e elevada bioatividade.* (Pôster)

d. Papers presented at national conferences;

“58º Congresso Brasileiro de Cerâmica, Bento Gonçalves, RS, de 18 a 21/05/2014.”

REVELO, R.J.; FERREIRA, E.B.; DIAS, L.L.; GOMES, K.R.; MENEGAZZO, A.P.; “*Reformulação de esmaltes cerâmicos a partir de vidros reciclados de Tubos de Raios Catódicos*”. (Pôster apresentado)

CESARINO, V.; FERRÃO, C.P.; SALOMÃO, R.; FERREIRA, E.B.; “*Precusores funcionalizantes de poros à base de gel de silicatos para obtenção de cerâmicas bioativas*”. (Pôster apresentado)

“XXXVII Encontro Nacional de Física da Matéria Condensada. Costa do Sauípe, BA - 12 a 16 de maio de 2014”

ZANOTTO, E. D. *Crystal nucleation in glasses, a 60-year perspective.* (Invited talk).

ZANOTTO, E. D. *Overview of the (UFSCar-USP-UNESP) center for glass research* (Invited talk)

Lima, M.; Nicola, V. O. M.; Tsuchida, J. E.; Rodrigues, A. C. M.; ZANOTTO, E. D.; Schneider, J. F.. *Study of mixed alkali effect on $x\text{Me}_2\text{O} \cdot (1-x)\text{Na}_2\text{O} \cdot \text{P}_2\text{O}_5$ ($\text{Me} = \text{K}, \text{Rb}$) glasses.* (Pôster)

DE CAMARGO, A. S. S. *Developments on new applications of vitreous and vitroceramic materials.* (Oral presentation)

GONÇALVES, T. S.; MOREIRA, R.; ECKERT, H.; DE CAMARGO, A. S. S.. *New fluoro-aluminophosphate glasses doped with Er^{3+} and Yb^{3+} - Structural and Optical Characterization.* (oral)

MATTOS, R.I.; TAMBELLI, C.E.; MAGON, C.J. ; DONOSO, J. P.; SALVI, D.T.B.; MESSADDEQ, Y.; RIBEIRO, S.J.L.. *TD-NMR Study of ionic conductor membranes based on bacterial cellulose.* Abstract 522-1 [POL] (Pôster)

MATTOS, R.I.; CAMARGO, R.A.G. ; PERICINI, H.A.; TAMBELLI, C.E.; RAPHAEL, E.; MAGON, C.J. ; DONOSO, J. P.; SANTAGNELI, S.H.; RIBEIRO, S.J.L.. *TD-NMR Study of chitosan Agar based biopolymer membranes.* Abstract 523-1 [POL] (Pôster)

“Annual Conference of the Brazilian Physical Society, May 2014.”

Eckert, H. *Composition/Structure/Property Correlations in Glasses and Glass Ceramics.*

Eckert, H. *The mixed network former effect in glasses: structure/property correlations in Phosphate-based glass systems.*

“II Seminário UEPG, Ponta Grossa, PR, 13-14 agosto de 2013”

ZANOTTO, E.D. *LaMaV / UFSCar - 36 Anos de Ensino, Ciência e Inovação*. (Opening Talk)

“IN 2013 – Latin American Osseointegration Congress, Expo Center Norte, São Paulo, Brasil - 25 a 28 de setembro, 2013”

CHINAGLIA, C. R.; PEITL, O.; SOUZA, C.W.O.; CAMPANINI, L.; ZANOTTO, E.D., *A New Bactericidal Titanium Surface with Low Contact angle and High Bioactivity*. (Pôster)

“XXI Congresso de Iniciação Científica da UFSCar, São Carlos, UFSCar - de 14 a 18 de outubro de 2013”

MACHADO, N. M.P., ZANOTTO, E. D., RODRIGUES, A. M. “*Paradoxo de Kauzmann-Uma abordagem*” (Pôster).

FERNANDES, B., ANDREETA, M. R. B., VILLAS BOAS, L. A. “*Síntese de Cerâmica de Lítio-Lantânio-Titânio-Oxigênio para aplicação na medição de pH*” (Pôster)

JESUS, I. R. F.; ANDREETA, M. R. B. “*Vidros e Vitrocerâmicas do sistema Li₂O - La₂O₃-TiO₂ - SiO₂*”.

“XXXVI Encontro Nacional de Física da Matéria Condensada, Águas de Lindóia, SP - maio 2013.”

MARCONDES, S.P. ; ANDREETA, M.R.B. ; HERNANDES, A. C. “*Development of crystalline Al₂O₃-Nd₂O₃ tips for application in thermotherapy*”. (Poster)

DE CAMARGO, A. S. S. *Optical materials based on Ir(III) complexes incorporated in mesoporous silicate hosts: In situ versus topotactic synthesis approaches and electronic structure analysis*. (oral presentation)

SILVA, I.D.A. ; DONOSO, J.P. ; C.J. MAGON, R.I. MATTOS, C.E. TAMBELLI, A. PAWLICKA, E. RAPHAEL. *Electron paramagnetic resonance of Cu(II) doped chitosan-based bio-membranes*. Abstract P210-1 [Pol]. (Poster)

SILVA, I.D.A. ; DONOSO, J.P. ; NASCIMENTO, O.R. ; ETCHEVERRY, S.B. *EPR study of the exchange and dipolar coupling in a copper dimer with santononic acid*. Abstract P210-2 [Mat]. (Poster)

SILVA, I.D.A. ; DONOSO, J.P.; MAGON, C.J. , LIMA, J.F. ; NALIM, M.; MONTESSO, M.; SIQUEIRA, R.F. . *Electron paramagnetic resonance study of antimony based glasses doped with Fe(III) ions*. Abstract P210-3 [Mat]. (Poster)

MATTOS, R.I.; GAZZOLA, M.R.B.; NASCIMENTO, D.D. ; TAMBELLI, C.E.; SANTAGNELI, S.H.; RIBEIRO, S.J.L.; MAGON, C.J.; DONOSO, J.P.. *NMR Spectroscopy of gelatin-chitosan blends*. Abstract P301-1 [Pol]. (Poster)

MATTOS, R.I.; TAMBELLI, C.E.; RAPHAEL, E.; VIEIRA, K. O.; SANTOS, H.F.; SCHIAVON, M.A.; MAGON, C.J. ; DONOSO, J. P. . *NMR Spectroscopy study of biopolymers doping with nano carbon tube functionalized CdTe quantum Dots*. Abstract P303-1 [Pol]. (Poster)

“XII Encontro da SBPMat, Campo do Jordão – SP, 2013.”

MARCONDES, S.P.; ANDREETA, M. R. B.; HERNANDES, A. C.; "Laser-Heated Pedestal Growth of $Al_2O_3-Nd_2O_3$ system for thermotherapy devices". Anais de Resumo, 2013. v. H-P18.

“1º Encontro de Ciência e Engenharia de Materiais de São Carlos: Energia, Sustentabilidade e Inovação, São Carlos – SP, Brasil - de 27 a 29 de Novembro de 2013”

ZANOTTO, E.D. - "A bright future for glass-ceramics" (invited)

ANDREETA, M. R. B.; JESUS, I. R. F.; ZANOTTO, E. D. "Estudo da produção vidros e vitrocerâmicas do sistema $Li_2O - La_2O_3-TiO_2 -SiO_2$ ".

BACHA, M.G.; BERTARINI, P.L.L.; FERREIRA, E.B.; "Sinterização de vidros com cristalização concorrente assistida por campo elétrico". (pôster)

BARROS, L.M.; FERREIRA, E.B.; "Concretos de alto desempenho a partir de matérias-primas amazônicas e cimentos vítreos", (pôster)

REVELO, R.J., PEGORIN, L.G.; CARDINALI, J.; FERREIRA, E.B.; "Reformulação de esmaltes cerâmicos a partir de vidros reciclados de Tubos de Raios Catódicos". (pôster)

FERNANDES, R.G.; FERREIRA, E.B.; "O efeito da forma de partículas de vidro na cinética de cristalização determinada por DSC". (pôster)

CESARINO, V.; SALOMÃO, R.; FERREIRA, E.B.; "Agentes porogênicos à base de gel de silicatos para obtenção de cerâmicas com poros funcionais" (pôster apresentado)

“Department of Chemistry, University of Sao Paulo, Riberão Preto, November 2013.”

ECKERT, H. *Modern Solid State NMR Strategies for the Structural Study of Disordered Materials.*

“I Workshop do Center for Research, Tecnology and Education in Vitreous Materials (CeRTEV), São Carlos, SP, 10/08/2013”

DE CAMARGO, A. S. S. *Materiais vítreos ópticos e luminescentes: Planejamento, síntese e caracterizações estruturais e fotofísicas.* (oral presentation)

FERREIRA, E.B.; "Innovation and tech transfer". (apresentação oral)

FERREIRA, E.B.; "O Grupo de Vidros e Vitrocerâmicas do Departamento de Engenharia de Materiais da EESC/USP". (apresentação oral)

MACENA, G.S.; FERREIRA, E.B.; "Cristalização e habilidade de formação de vidros no sistema $CaO.SiO_2-Na_2O.2CaO.3SiO_2-Na_2O.3CaO.6SiO_2$ ". (apresentação oral)

CESARINO, V.; FERREIRA, E.B.; "Precusores funcionalizantes de poros a base de gel de silicatos para vitrocerâmicas" (apresentação oral)

MAGON, C.J. ; DONOSO, J. P. *CW and pulsed EPR as a tool to characterize glass and glass ceramics.* (oral presentation)

In this meeting all researchers and ~50 students and post-docs of the CeRTEV presented a summary of their research work.

“XII Encontro da SBPMat, Campos do Jordão -2013”

BOTELHO, M. ; QUEIROZ, T. B. ; de Camargo, A.S.S. . *New approaches towards optical materials based on coordination metal complexes and organic dyes incorporated in sol-gel mesoporous hosts*. Livro de resumos, 2013. (oral presentation)

“III Simpósio sobre resíduos sólidos – III SIRS (2013), do Núcleo de Estudo e Pesquisa em Resíduos Sólidos da USP-São Carlos, São Carlos, SP, de 02 a 04/12/2013.”

REVELO, R.J.; FERREIRA, E.B.; BRANDÃO, D.; RAGONESI, R.; “*Reciclagem do vidro de monitores de tubo de raios catódicos*” (pôster)

“I Workshop Bionetec, São Carlos, SP, 22/11/2013.”

FERREIRA, E.B.; “*O Grupo de Vidros e Vitrocerâmicas do Departamento de Engenharia de Materiais da EESC/USP*”, apresentação oral.

CESARINO, V.; SALOMÃO, R.; FERREIRA, E.B. “*Agentes porogênicos à base de gel de silicatos para obtenção de cerâmicas com poros funcionais*”, apresentação oral.

“16th Brazilian Workshop on Semiconductor Physics, Itirapina, SP, May 05-10, 2013”

RINO, J. P. “*Barium Sulfide: A Molecular Dynamics Simulation*”. (Oral presentation)

“IV Simpósio de Biotecnologia da UFSCar, São Carlos – SP, 2013.”

CAMPANINI, L. A.; SOUZA, C.W.O.; PEITL, O.; CHINAGLIA, C. R.; SOUZA, M. T. *Análise da atividade bactericida de um vidro bioativo na forma de fibras e de pó para aplicações médicas e odontológicas*. (Pôster)

Mini Curso ministrado:

RINO, J. P.; *Simulação Computacional: Dinâmica Molecular*
IX Semana de Física da UFSCar - IXSEFIS
Universidade Federal de São Carlos, São Carlos, SP
Ano: 2013

RINO, J. P.; *Dinâmica Molecular: uma breve introdução*
XVIII Encontro Sergipano de Física
Universidade Federal de Sergipe, Aracaju, SE
Ano: 2013

e. Requested or obtained patents;

GALLO, L. S. ; RODRIGUES, A. C. M. ; ZANOTTO, E. D. ; PEITL FILHO, O. . COMPOSIÇÕES VITROCERÂMICAS, VITROCERÂMICAS OBTIDAS, ARMADURA DE SACRIFÍCIO E ARTIGO

PARA PROTEÇÃO BALÍSTICA. 2013, Brasil.

Patente: Privilégio de Inovação. Número do registro: BR10201301776, data de depósito: 26/06/2013, título: "**Composições Vitrocerâmicas, Vitroceâmicas obtidas, Armadura de Sacrifício e Artigo Para Proteção Balística**", Instituição de registro: INPI - Instituto Nacional da Propriedade Industrial.

ZANOTTO, E. D.; SOUZA, M. T. e PEITL FILHO, O. Composição vítrea, fibras e tecidos vítreos bioativos e artigos, 2013.

REQUERIDA Aguardando Exame do INPI (que pode levar de 7 a 10 anos a contar da data de depósito da patente). Em 2014 será realizado a deliberação para depósito PCT. Pagamento da 3ª anuidade será efetuado em 2015. Publicação de depósito de patente publicado na RPI em 13/05/2014. Pedido disponível para ser inserido no Lattes.

ZANOTTO, E. D.; CHINAGLIA, C. R.; PEITL FILHO, O. "Processo de recobrimento descontínuo utilizando um biomaterial bioabsorvível e bioativo aplicado sobre substratos sólidos, recobrimento descontínuo e seu uso". 2014 Brasil.

REQUERIDA Aguardando Exame do INPI (que pode levar de 7 a 10 anos a contar da data de depósito da patente) Em 2015 será realizado a deliberação para depósito PCT. Pagamento da 3ª anuidade será efetuado em 2016. Publicação de depósito de patente publicado na RPI em 05/03/2014 exigência formal em 29/04/2014 (exigência formal é exigência voltada a parte administrativa, dessa forma a Agência está se posicionando frente ao INPI). Pedido disponível para ser inserido no Lattes.

f. Chapters of books published;

PEITL, O.; ZANOTTO, E.D. ; SERBENA, F.C. ; HENCH, L.L. . Bioactive glass-ceramics for load-bearing applications. An Introduction to Bioceramics. 2ed.: World Scientific Publishing Company, 2013, v. 2, p. 1-9.

FOKIN, V. M.; CABRAL, A. A. ; REIS, R.C.V.M. ; **ZANOTTO, E.D.. Comments on DTA/DSC Methods for Estimation of Crystal Nucleation Rates in Glass - Forming Melts**. In: Sesták, Jaroslav; Simon, Peter. (Org.). Thermal analysis of Micro, Nano- and Non-Crystalline Materials. XXId.: Springer, 2013, v. 9, p. 325-351.

H. ECKERT, S.J.L. RIBEIRO, S. H. SANTAGNELI, M. NALIN, G. POIRIER, Y. MESSADDEQ, Glasses on the Nanoscale , Handbook of Nanomaterials, R. Vajtai, ed. Springer-Verlag Berlin, 665-692 (2013).

CARDOSO, C. A. ; SERGEENKOV S. ; **ANDREETA, M.R.B. ; HERNANDES, A. C. ; LEITE, E. R. ; LIMA, O. F. ; ARAUJO-MOREIRA, F. M. "Growth, Characterization and Magnetic Properties of Polycrystalline Fibers of Electron Doped Manganites"**. In: Lixin Yu. (Org.). Doping: Properties, Mechanisms and Applications. 1ed.: Nova Science Publishers, v. 1, p. 71-80, 2013.

g. Books published with team members as author, editor or organizer;

ZANOTTO, Edgar Dutra . **CRYSTALS IN GLASS - A Hidden Beauty**. New Jersey: John Wiley & Sons & The American Ceramic Society, 2013. v. 1. 110p . ISBN: 9781118521434

RINO, José Pedro; COSTA, Bismarck Vaz da. **ABC da Simulação Computacional**. São Paulo: Editora Livraria da Física, 2013. 192 p. ISBN 9788578612030 EAN 9788578612030

h. Dissertations (MSc) defended;

Name: Igor d`Anciães Almeida Silva

Advisor: José Pedro Donoso

Title: Estudos de ressonância paramagnética eletrônica de complexos mononucleares e dinucleares de cobre - Instituto de Física de São Carlos (IFSC), Universidade de São Paulo (USP) 16 de fevereiro 2014

Name: Tássia de Souza Gonçalves

Advisor: Andrea S. S. de Camargo

Title: Caracterização estrutural e espectroscópica de vidros fluorofosfatos dopados e co-dopados com Er^{3+} e Yb^{3+} - Instituto de Física de São Carlos – IFSC/USP, Maio de 2014.

Name: Raphaell Junnio Moreira,

Advisor: Hellmut Eckert

Title: Structural Characterization of Fluorophosphate Glasses Using NMR Methodologies - IFSC-USP May 2014.

Name: Melanie Siedow

Advisor: Hellmut Eckert

Title: Solid State NMR spectroscopic studies on frustrated Lewis pairs - WWU Münster, June 2014

i. Thesis (PhD) defended;

Name: Daniel Roberto Cassar

Advisor: Edgar Dutra Zanotto

Title: Diffusion, crystallization, viscous flow and relaxation kinetics in diopside and lithium diborate glasses. 2014. 176 f. Tese (Doutorado) - Departamento de Engenharia de Materiais, Universidade Federal de São Carlos, São Carlos, 2014.

Name: Alisson Mendes Rodrigues

Advisor: Edgar Dutra Zanotto

Title: Processos difusionais, cristalização e escoamento viscoso em disilicato de bário vítreo. 2014. 202 f. Tese (Doutorado) - Departamento de Engenharia de Materiais, Universidade Federal de São Carlos, São Carlos, 2014.

Name: Mariana Carlos de Oliveira Villas Bôas.

Advisor: Edgar Dutra Zanotto

Title: Desenvolvimento e Caracterização de vitrocerâmicas do sistema $\text{Li}_2\text{O-SiO}_2$ para aplicação odontológica. Tese (Doutorado em Programa de Pós Graduação em Ciência e Engenharia de Materiais) - Centro de Ciências Exatas e de Tecnologia, Fundação de Amparo à Pesquisa do Estado de São Paulo. 2013.

Name: Clever Chinaglia.

Advisor: Edgar Dutra Zanotto

Title: O uso de um vidro altamente bioativo para a melhoria da bioatividade da superfície do titânio - desenvolvimento de um método para recobrimentos descontínuos. Tese (Doutorado em Ciência e Engenharia de Materiais) - Universidade Federal de São Carlos, Conselho Nacional de Desenvolvimento Científico e Tecnológico. 2013.

Name: José Luis Narváes Semanate

Advisor: Ana Candida Martins Rodrigues

Title: Caracterização elétrica e microestrutural de vitrocerâmicas condutoras por íon lítio com estrutura Nasicon. Tese (Doutorado em Programa de Pós Graduação em Ciência e Engenharia de Materiais - UFSCar) 2013

Name: Murilo Camuri Crovace.

Advisor: Ana Candida Martins Rodrigues

Title: Scaffolds vitrocerâmicos obtidos via prototipagem rápida aplicáveis à medicina e odontologia. Tese

(Doutorado em Programa de Pós Graduação em Ciência e Engenharia de Materiais) - Centro de Ciências Exatas e de Tecnologia, Fundação de Amparo à Pesquisa do Estado de São Paulo. 2013.

Name: Rolando Placeres Jimenez

Advisor: José Pedro Rino

Title: “Dielectric and elastic response of perovskites: Modeling and simulation” (Pós-Doutorado em Programa de Pós Graduação em Física – UFSCar) 2013.

Name: Thomas Wiegand,

Advisor: Hellmut Eckert

Title: *Structure, Reactivity and Cooperativity of functional organo phosphorus compounds: Development and Application of Modern Solid State NMR and DFT Strategies*, Dr. rer. nat. Physical Chemistry - Westfälische Wilhelms Universität Münster, July 2013.

Name: Frederik Behrends,

Advisor: Hellmut Eckert

Title: *Magnetic Resonance Spectroscopy of paramagnetic functional materials*. Dr. rer. nat. Physical Chemistry - Westfälische Wilhelms -Universität Münster, July 2013.

Name: Zhaoyang Zeng,

Advisor: Hellmut Eckert

Title: *Synthesis and Characterization of Hybrid Materials based on the Intercalation of paramagnetic guest species into inorganic host lattices*, Dr. rer. nat. Physical Chemistry – Westfälische Wilhelms-Universität Münster, December 2013.

Name: Cornelia Schröder,

Advisor: Hellmut Eckert

Title: *Modern Solid State NMR Studies for the Characterization of Lithium Containing Glasses and Glass Ceramics*, Dr. rer. nat. Physical Chemistry – Westfälische Wilhelms-Universität Münster, January 2013.

Name: Maturi Ilibi

Advisor: Hellmut Eckert

Title: *Intercalation of luminescent Eu(III) complexes into mesoporous silica MCM-41*, Dr. rer. nat. Physical Chemistry – Westfälische Wilhelms-Universität Münster, March 2013.