

**ESF Exploratory Workshop (ref. EW06-087)**

*"Glassy Liquids Under Pressure: Fundamentals and Application"*

Ustroń (Silesia Region), Poland, 11-13 Oct. 2007

## Scientific Report

**Web page:** <http://www.us.edu/universytet/konferencje/drozd-rzoska/>

**Web page:** <http://www.esf.org/activities/exploratory-workshops/workshops-list/workshops-detail.html?ew=4771>

Convenors:

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## **1. Executive Summary:**

The organizers of this ESF EW were Dr. Aleksandra Drozd-Rzoska (*convenor*) (Silesian University, Poland) and Prof. Josep Lluís Tamarit (*co-convenor*), (ETSEIB, Spain).

During the Workshop the organizational issues associated with the conference desk and technical issues related to subsequent lectures were supported by Prof. Sylwester J. Rzoska, dr. Michał Mierzwa and Kamil Kamiński (PhD) from the Silesian University.

### **1.1 Conference loci & accomodation**

The ESF Exploratory Workshop on "Glassy Liquids under Pressure: Fundamentals and Application" was held in Ustroń, from 11<sup>th</sup> to 13<sup>th</sup> October, 2007. Ustroń is a picturesque village located in Beskidy Mountains, 60 km from Katowice – the capitol of the Silesian Region (Poland) – the loci of the Silesian University. The ESF EW was arranged in Hotel Jaskółka in Ustroń, which offered a superior 4-star standard for the 3-star prize. The conference site was located in the heart of Beskidy Mountains, with beautiful view on surrounding hills. Ustroń is known as tourist and recovery resorts, focused on heart and rheumatic diseases. Participants met at the evening 10<sup>th</sup> Oct. in the Institute of Physics, Silesian University and next they moved to the conference loci by a special bus. At 14<sup>th</sup> Oct. 2007, morning the same bus moved participants of the ESF EW from the conference loci to the Katowice-Pyrzowice Airport and to the centre of Katowice. Each participant obtained a Workshop Bag with logos of the ESF, Silesian University and ETSEIB, containing a pen, pencil, markers and a notebook.

### **1.2 General comments about the ESF EW**

27 researchers from 16 countries presented lectures related to various the pressure induced vitrification in variety of soft materials, ranging from low molecular liquids, resins, polymers to liquid crystals, plastic crystals and bio-liquids. Lectures were related to up-to-date experimental results, theoretical & numerical issues as well as applications. The brainstorming discussion outlined the research required for the progress in the field of glass transition possible due to the application of pressure up to its challenging limits. It was a comprehensive mix of topics between theoretical, numerical and experimental research. Emerging applications in geophysics, modern materials engineering, pharmaceutical and food industry were also presented.

Lectures and discussions were arranged in subsequent days in following panels – general topics:

- (i) Glassy Liquids under Pressure: General Issues
- (ii) Liquid–Liquid Transition, Pressurization & the Glass Transition Puzzle
- (iii) Vitrification under Pressure: New Opportunities

Each presentation was limited to 35 minutes, including discussion. Brainstorming discussions were continued during long time coffee breaks, at the dinner break and during evening discussions. The latter were facilitated by social events. A permanent poster session was arranged, to introduce additional artifacts supporting discussions.

A number of comments was made at the time of the workshop and afterwards to the effect that participants strongly valued the level of the discussion and the manner in which debates/discussions took place. This includes the relaxing atmosphere matched with high quality intensive scientific programme. The superior quality of the accommodation and food, extraordinary arrangements of refreshments for coffee breaks and the “free” debate time was stressed. For each evening an impressive social event, to create interpersonal links was arranged. Finally, participants appreciated the fact that organizers took care for all participants from the moment of their arrival to Poland until leaving after the ESF EW.

### **1.3 Publicity**

- (a) Information about the Workshop was available at the WEB page of the ESF as well as the special page prepared by Aleksandra Drozd-Rzoska. At the latter post-ESF EW photos are also shown
- (b) Links to these pages are available at official pages of the Silesian University (Poland) and ETSEIB (Spain)
- (c) Before the ESF EW a note describing the ESF and announcing the ESF “*Glassy Liquids under pressure*” was available (in polish) at the official page of the Silesian University
- (d) An article the “*Gazeta Uniwersytecka*” – the monthly journal of the Silesian University society describing the meeting “The mystery of the transition to the glassy state” (english translation) was prepared by Aleksandra Drozd-Rzoska. It recalls also ESF in general, contains ESF logo as well three photos from the workshop.
- (e) In the Institute of Physics, Silesian University (Poland) and subsequently at the conference loci in Ustroń two types of posters (in A0 and A1 formats) additionally disseminated the knowledge of the ESF EW. They contain logos of the ESF, Silesian University (Poland) and ETSEIB (Spain)

- (f) a unique publicity, important for the glass transition focused researchers in general, will be the special issue of the Journal of Physics: Condensed Matter "Glassy Liquids under Pressure".

## 2. Scientific content of the Event

The elucidation of the origin of the dramatic slowing down of the relaxation times of a system as it approaches the glass transition has been recognized as the one of 6<sup>th</sup> greatest challenges of the XXI century of the condensed matter physics and material engineering in the ranking of the "Science" journal. This issue is not only of fundamental interest but has also several technologically important aspects

The ESF EW "Glassy liquids under pressure: Fundamentals and Applications" brought together the outstanding members of the European research groups dealing with the vitrification phenomenon and pressure. Recent pressure experiments employed by different groups, also forming by participants of this ESF, made it possible to provide the first ever quantitative assessments of the key parameters controlling the glass transition. From the experimental side this was due to the far reaching challenging domains, from negative pressures up to extremely highly pressures (in the GPa range), linked with sophisticated modern techniques.

The ESF EW began from introductory remarks describing the history and current tasks of the European Science Foundation and ESF Exploratory Workshop. This topic was prepared by the Josep Lluís Tamarit (ETSEIB, Barcelona, Spain), the co-convenor.

Subsequently, the first day discussions of the ESF EW focused on the topic:

*"Glassy Liquids under Pressure: General Issues".*

Following lectures were presented:

1. **Kia L. Ngai** (Naval Res. Lab., Washington DC, USA/UnivesrItaly): *"Significant Impact of Pressure Studies on Fundamental Understanding of Glass Transition: Theory and Experiments"*.

Remarkable properties of glass-forming which have been recently discovered by the application pressure were discussed. Particularly, novel findings associated with sources of the secondary relaxation and the application of Coupling Model were recalled. The evidence collected so far indicated that the ultimate theory for the glass transition should take into account results of pressure studies, the link between the Johari – Goldstein relaxation and the coupling model as well as the heterogeneous dynamics.

*In the subsequent discussion it was stressed that although high pressure studies showed that only the comprehensive pressure and temperature data can serve as a tool for the verification of theoretical models - the increasing of high pressures may yield even more reliable data here. On the other hand extreme pressures in the GPa domain shows some new features, beyond presented facts.*

2. **Vadim Brazhkin** (Russia): "Puzzling Behaviour of Liquids at multi-GPa Pressure Range: Recent Examples".

The issues of the extrapolation to multi-GPa pressures of the experimental data obtained at moderate pressures were considered for different classes of glass-forming substances. For covalent glass-forming substances, the phase transitions and structural changes are major factors that hamper extrapolation. Organic glass-forming liquids are not ground thermodynamic states of the matter: under high pressures they transform to the polymeric substances and then to the mixture of simple inorganic compounds. Therefore, the extrapolation of the data obtained at moderate pressures is hardly possible for this class either. Metallic melts and rare-gas liquids are the only substances whose properties can be extrapolated into the megabar region. However, such an extrapolation is highly uncertain due to the low viscosity and weak pressure dependences of the properties of these liquids. New experimental studies of rare-gas and metallic liquids in the pressure region of tens of GPa are urgently needed for the extrapolation to be reliable.

*In the subsequent discussion* the extreme pressure domain was indicated as particularly interested domain for future studies on vitrification. Isak Avramov pointed out some possibilities of his recent findings for the analysis of some of results presents. Particular interest attracted experimental solutions enabling measurement of physical properties in the multi-GPa domain.

3. **Isak Avramov**, (Bulgaria): "Pressure Dependence of Viscosity or is the Earth Mantle a Glass?".

First it was recalled that little is known about the real condition in the Earth interior because direct sampling is not feasible. The propagation of seismic waves is the only instrument to investigate the mantle. Therefore viscosity  $\eta$  is of prime importance. Experimental data indicate that it is about  $10^{22}$  Pa.s. At so high viscosity even molten materials behave solid like. The aim of the present lecture was to demonstrate that, due to the extreme pressure, viscosity increases sharply. In this way the glass transition temperature increases faster than the melting point, so an important part of the mantle could be in a glassy state, although being molten.

*In the subsequent discussion* problems of the so called Avramov model for portraying the viscosity evolution and the glass temperature evolution for the deep Earth structures analysis were recalled. S. J. Rzoska indicated the role of the possible "reverse" melting and vitrification at extreme pressures. Vadim Brazhkin pointed out the significance of the appearance of new structures, including pressure induced polymerization, not included into the presented model.

4. **Thomas Voigtmann** (U.K.): "Glasses under High Pressure a Mode-Coupling Perspective".

The role of the energy and the entropy for vitrification in glass forming systems was worked out. The analysis based on the comparison of classical, low-molecular glass formers and colloidal glass. The pressure dependence of the glass temperature was pointed out as the key artefact enabling the comparison between these two system. The density driven transformations were suggested for  $P > 1$  GPa. It was stated that colloidal glasses show the same trends as fragile low "classical" glass formers.

*In the subsequent discussion* questions associated with taking into account the reversal of vitrification, observed in colloids were the key point. In following prediction of the mode coupling theory for the pressure studies were pointed out as the important point for future studies.

5. **Marian Paluch** (Poland) "Thermodynamical Scaling in Glass-Forming Liquids".

Recent empirical finding for the scaling of temperature and pressure dependences of dielectric relaxation times into the volume related paths were summarized. These included dependences introduced by Mike Roland et al. and Christianne Alba-Simionesco et al. Presented novel experimental result covered the unexplored so far pressure domain, extending well above 1 GPa.

*In the subsequent discussion* the question of the validity of this scaling for glass formers with different types of molecular interaction was extensively discussed. The next issue recalled its validity in the extreme pressures domain.

6. **Ulrich Buchenau** (Germany): "Dielectric Relaxation in Molecular Glasses".

The lecture focused on properties of vitrifying liquids emerging when carrying out dielectric relaxation and mechanical relaxation experiments. The difference in time scales, some shifts in the manifestation of the secondary relaxation and different activation barriers were pointed out. The anal analysis recalled the recently developed analysis based on the Eshelby model.

*In the subsequent discussion issues associated with the experimental insight based on mechanical relaxation under pressure, in practice not available so far were discussed.*

7. **Gabriel Cuello** (France): "Structure of Amorphous Materials : Neutron diffraction".

New possibilities offered by structural pressure studies of amorphous materials in the Laue – Langevin Institute (France) were shown. This included the outline of the theoretical background and the presentation of the main facilities. Finally, the application of the neutron diffraction for several examples of amorphous materials was shows

*In the subsequent discussion mainly question related to current possibilities of implementing the high pressure technique were formulated.*

8. **Alberto Rivera** (Spain): "Electric Response of Room Temperature Ionic Liquids under Pressure".

Studies of relaxation spectra of the ionic glass forming liquid 1-butyl-1-methylpyrrolidinium bis[oxalato]borate (BMP-BOP) were presented in a wide temperature and pressure range. The similarity to the behaviour of "normal" glass formers was notified. It was found that even the elevated pressure can separate the secondary relaxation on the high frequency flank of the primary relaxation. The application of the Ngai coupling model was shown.

*In the subsequent discussion it was stressed that results presented are probably the first report on pressure "dynamic" studies in a glass forming ionic liquid. Kia Ngai discussed novel possibilities emerging for his coupling model in "ionic glasses". Issues related to the control of the strength of the interaction, hardly possible in other systems, were discussed.*

9. **Simone Capaccioli** (Italy): "Interdependence of Primary and Secondary Relaxations under Pressure and Temperature Variations in Glass Forming Systems".

The lecture outlined problems associated with the secondary (Johari-Goldstein) and primary and secondary relaxations in supercooled and superpressed liquids. Particular attention was paid to the effect of pressure on secondary relaxation and excess wing. The analysis extensively recalled the Ngai's coupling model. Finally, the issue of superscaling of  $\tau_\alpha(\rho, P)$  and  $\tau_\beta(\rho, P)$  were discussed

*In the subsequent discussion the success of the Coupling Model was first stressed. Next problems remaining for the superscaling, partially associated with searching the ultimate parameterization of the pressure dependence of the glass temperature were discussed.*

10. **Sylwester J. Rzoska** (Poland): "Direct Insight into Heterogeneous Dynamics from the Nonlinear Dielectric Spectroscopy".

Recently, the nonlinear dielectric spectroscopy (NDS) was suggested as the successor of the broad band dielectric spectroscopy for studying the vitrification phenomenon. This is related to the fact that NDS is directly linked to the 4-point correlation function. The lecture recalled these issues and presented key experimental solutions for NDS measurements. Next, results of the first ever frequency selective NDS measurement using dual-field and modulation domain technique were presented in supercooled and superpressed dibutyl phthalate and epoxy resin DGEBA

*In the subsequent discussion it has been stated that NDS may be the most important methods for future studies on the glass transition. The single-exponential decay of the selective burst was indicated as the evidence for the so called homogeneous scenario.*

The second day discussions of the ESF EW focused on the topic:  
"Liquid-Liquid Transition, Pressurization & the Glass Transition Puzzle".

The discussion was arranged by following lectures:

11. **Mark Wilson** (U.K.): "Evidence for Polyamorphism from Computer Simulation"

The development of simple models paralleling length and time scale evolution in polyamorphic and vitrifying systems, with the possible relationship with experiments was discussed. Systems of interest included MX<sub>2</sub> network liquid, Silicon and Y/Al oxides. The analysis was associated with the selection of basic potentials for model systems

*In the subsequent discussion possible further correlation between experiments and presented numerical model analysis, particularly regarding the pressure evolution of the glass temperature. Subsequently experimental manifestations of predicted hallmarks of polyamorphism. Finally, hints to glass-forming ability emerging in model systems were recalled.*

12. **Martin Wilding** (U.K.): "Fragility, Polyamorphism and Amorphous Structure: Neutron Diffraction studies of Silicate Glasses at High Pressure".

Results of in situ neutron diffraction studies performed in two glass forming silicate systems, a fragile magnesium silicate and vitreous silicate were presented. These data demonstrated the structural changes that occur as amorphous materials are compressed. These experiments showed changes in the mid and intermediate-range order that can be correlated in theology. These changes in structure are between w.0 and 4.0 Angstrom in real space over the pressure up to 24 GPa. The diffraction identified trends in structure, although some puzzle remained due to complicated background.

*In the subsequent discussion it was pointed out that these experiments illustrated the richness of high pressure induced polyamorphism and structures as well as opportunities that the development of new neutron facilities and instruments offer to explore the connection between structure and fragility.*

13. **Jeppé Dyre** (Denmark): "One or More Order Parameters: The High-Pressure Perspective".

First, arguments that the vast majority of glass-forming liquids require more than one "order" parameter were summarized. Recent experimental findings were subsequently recalled. *It was shown that a single "order" parameter description applies to a good parameterization whenever thermal equilibrium fluctuations of fundamental variables are strongly correlated. This was supported by results of the computer simulation. Finally a new conjecture to which experiments at varying temperature (T) and pressure (P) follows the density ( $\rho$ ) scaling expression  $\tau(P, T) \approx F(\rho^* T)$  if and only if the liquid is strongly correlated was stated*

*In the subsequent discussion the significance of theoretical defining conditions of the empirical (so far) scaling P and T dynamic data was stressed. It was recalled that this empirical scaling is as one of the most important experimental findings for the glass transition phenomenon in the last years.*

14. **Marie-Claire Bellisant-Funel** (France): "Influence of Pressure on Water-Biomolecules Systems. Applications for Food Industry".

Investigations of structure and nanosecond dynamics of the interfacial water from 77 K to 280 K were presented. Results presented mainly based on combined inelastic neutron diffraction combined with DSC results. A water monolayer absorbed on the hydrophilic surface of Vycor was considered as a model system. Finally, practical conclusions for the modern way of the food conservation were outlined.

*In the subsequent discussion the clear glassy features of the interfacial water were stressed. Strong correlation between the onset of protein dynamics and interfacial water rotational motion. The correlation between the onset of the dynamics of proteins and the interfacial rotational motion was pointed out.*

15. **Victor Teboul** (France): "Dynamical Heterogeneity in Supercooled Water" the Effect of Confinement and Pressure".

Recent experimental and theoretical findings associated with studies on confined water were presented. Particular attention was paid to the fragile to strong crossover. The application of confinement made it possible to identify the length scale of dynamic heterogeneities.

*In the subsequent discussion it was stressed that the presented experimental evidence linking pressure and confined water is at very beginning. It was also suggested that joining pressure and confinement may led to the verification of some "negative pressure like" feature of the confinement.*

16. **Giancarlo Franzese** (Spain): "Dynamics of Supercooled Liquid Water: Novel Pressure Effects".

Recent findings associated with second, liquid – liquid, critical point were outlined. Particular attention was paid to the estimation of the loci of the spinodal curve in the P- T plane, terminated with the critical point. Model based numerical analysis revealed glassy dynamics related to the appearance of bond – ordering nanostructures.

*In the subsequent discussion the issue of the experimental verification of the presented model predictions from pressure - temperature measurements were the key point. Particularly, possibilities of BDS or methods directly linked to fluctuations were discussed.*

17. **Ove Andersson** (Sweden): "Production and Investigations of Amorphous States by Means of High Pressure".

Results associated with the application of pressure up to 1.5 GPa on various systems, based on dynamic(dielectric relaxation) and thermodynamic measurements were presented. Particular attention was paid to the pressure induced amorphous states of water. The phenomenon of the pressure induced amorphization was analyzed basing on results presented. The appear of both stable and unstable phase was pointed out under extreme pressures.

*In the subsequent discussion the issue of the behaviour of the glassy water was the key point. Particularly the case of so called ice VI and ice XII was recalled*

18. **Juergen Horbach** (Germany): "Amorphous Silica under Pressure: A Computer Simulation Study".

First basic artefacts for the dynamics of silica glasses under pressure were recalled. Subsequently, possibilities of the molecular dynamics (MD) and of the mode coupling theory (MCT) for the model simulation analysis were discussed. In summary the maximum of diffusion around 20 GPa related to structural changes of the network was predicted

*In the subsequent discussion the issue of the range of validity of MD and MCT in silica glasses attracted attention. Next, the extension of results obtained for non-network glasses was discussed.*

19. **Victor Mazur** (Ukraine): "Two-Fluid Model of Glassy Liquids".

The possibility of building a general model for liquids basing on so called Pareto analysis, applied so far in economical sciences, was discussed. This led to the classical theory of phase transition and polymorphisms. It was stressed that this approach is at very beginning

*In the subsequent discussion some criticism for the validity of the presented approach for glassy and polymorphic systems appeared (J. Thoen). However, the emergence of two-fluid states was pointed out as an interesting artefact.*

20. **Jerzy Ziolo** (Poland): "Liquid-Liquid Transition in a Simple, One Component and Non-Mesogenic Liquid".

Novel experimental results for liquid-liquid transition in nitrobenzene and trans-dichloroethane were presented. For the latter the mentioned phenomenon was found well



above the melting temperature. For nitrobenzene anomalous increase of the strong electric field related nonlinear dielectric effect in the weakly supercooled state was reported. The phenomenon was explained by the appearance of the quasi-nematic nanostructure.

*In the subsequent discussion the novelty of the reported phenomenon was highlighted. The phenomenological model by Jean Hanus and to the general model for the liquid-liquid transition was pointed out.*

The third day of the ESF EW was related to the topic:  
"Liquid-Liquid Transition, Pressurization & the Glass Transition Puzzle".  
The discussion was arranged by following lectures:

21. **Attila Imre** (Hungary): "Fragility of Liquids, Solids and Glasses".

The issue of the negative pressure (isotropically stretched liquid) states and its relationship to the stable states under hydrostatic pressure were first shown. Next, experimental methods for inducing negative pressure states were discussed. Finally, novel experimental findings enabling parameterization of dynamic properties both in the pressure and temperature states were shown.

*In the subsequent discussion it was concluded that hydrostatic pressure studies in liquids are in a natural way extended in the negative pressure states. This defines the significance of negative pressures for vitrifying liquids. The still existing experimental challenge was recalled*

22. **Josep Ll. Tamarit** (Spain): "High Properties Inferred from Normal-Pressure Properties".

Phase equilibria in two-component systems sharing compounds from the series  $\text{CCl}_{4-n}\text{Br}_n$ ,  $n = 0, \dots, 4$  were analyzed focusing on experimentally non-available phase transitions. To reach this target the concept of isodomorphism was considered. The obtained thermodynamic properties were used to build up the topological pressure – temperature phase diagrams of the compounds within the series.

*In the subsequent discussion the impact of some peculiar points, including phase transition on properties under atmospheric pressure was stressed. The question arises if the present vice-versa way of prediction of the behaviour hidden under pressure from tests under atmospheric pressure is general or restricted to the given system or more general to some orientationally disordered crystals systems*

23. **Phil Salmon** (U.K.): "Structure of Tetrahedral Glass Forming Systems: from Ambient to High Pressures".

Neutron diffraction in AX<sub>2</sub> network glasses have shown that there are two length scales for network glasses at distances greater than the nearest neighbour. It was shown that the intermediate time scale is associated with the FSDP and the extended range order is related to the principal peak. The latter is expected from an analysis of the Ornstein – Zernike equations for simple model pair-potential and described by the ultimate decay of pair correlations.

*In the subsequent discussion the role of the competition existing between the ordering and the increased density was indicated. Questions for the link to the dynamics of low molecular weight glasses appeared. The latter seemed to be puzzling.*

24. **Jan Thoen** (Belgium): "Thermal and Dielectric Spectroscopy of Glass Forming Liquids and Confinement Effects".

Effects of the confinement on n-alkylcyanobiphenyl liquid crystals were discussed. The discussion recalled aerosil nanonarticles and Vycor porous glass. Based on BDS measurements the evolution of the bulk and surface related relaxation time was discussed. For the former the VFT and for the latter the Arrhenius dependence were notified. It was also pointed out that the disorder drives the relaxation time towards a more isotropic value.

*In the subsequent discussion the relationship between the confinement and pressure studies was pointed out. Attila Imre suggested the relationship to negative pressure (stretched liquids) states. Further, new and almost unexplored so far possibilities of linking high pressure and confinement in glass formers were discussed.*

25. **Samo Kralj** (Slovenia): "Influence of Nano-Particles on Phase and Structural Properties of Liquids Crystals".

The influence of nanoparticles on liquid crystal ordering was discussed, focusing on some universal features of the isotropic – nematic transition. Using the semi-microscopic lattice model and Brownian molecular simulation it was shown that after a quench from the isotropic phase a quasi stable domains forms. A Landau-type free energy expression was derived. It was shown that the resulting behaviour show the slave-master behaviour when pressure or temperature is varied.

*In the subsequent discussion issues related to the experimental verification of theoretical predictions proposed were considered. The question arised for the appearance of similar structures in non-mesogenic glass formers after the temperature or pressure quench.*

26. **George Floudas** (Greece): "Glass Transition in Discotic Liquids Crystals - Effects of Pressure".

The molecular dynamics of discotic liquid crystalline hexa-*peri*-hexabenzicoronenes (HBC-C<sub>10.6</sub> and dHBC-C<sub>14.10</sub>) with long alkyl side chains branched at the close vicinity of the HBC aromatic core by broad band dielectric spectroscopy was discussed. For both compounds a weak dipolar relaxation described by a VFT equation and the same glass temperature was reported. It was associated with the freezing of the on-plane disc rotation. The oxidation was identified as the dipole moment association source.

*In the subsequent discussion the significance of studying vitrification in experimental model system with well defined geometry was stressed. Some question were related to the possibility of the application of the recent density driven scaling, enabling the common representation of pressure and temperature data. The question also appear of the validity of the MCT description for vitrifying discotic liquid crystals.*

27. **Aleksandra Drozd-Rzoska** (Poland): "Glassy Dynamics in Rod-Like Liquid Crystalline Compounds".

Results on dynamics on rod-like nematic liquid crystals in the isotropic ("fluidlike") phase, consider as the experimental model system enabling decoupling of orientational and translational degrees of freedom were presented. The analysis based on of dielectric relaxation times was based on the recently introduced linearized derivative-based analysis.

*In the subsequent discussion the validity of the Mode Coupling Theory description was pointed out as the important artifact. However, the evidence of the value  $n \rightarrow -1/2$  for the "Jonsher" coefficient describing the high frequency wing within the series of n-cyanobiphenyls attract particular attention, due to its clear correlation to the finding of Jeppe Dyre who suggested this as a universal behaviour on approaching the glass transition.*

### **3. Assessment of results of the ESF EW**

#### **3.1 Contribution to the future direction of the field**

For some part of participants of this ESF EW it was the first possibility to get known and exchange opinions with others working in this field.

Several new objectives for further studies were identified.

First, they were associated with two domain, which studies just began, namely:

- a) The "new land" of extremely high pressure in the GPa domain
- b) The "new land" of negative pressures

Second, new objectives were associated with the association of high pressures with just developed, state-of-the-art experimental techniques. The nonlinear dielectric spectroscopy, neutron diffraction and nano-constraint are here the best examples

Third, new objectives associated with novel systems hardly explored so far. For instance: some bio-liquids, liquid crystals or plastic crystal. For these systems vitrification is often linked to a liquid-liquid transition.

Finally, new objectives created the influence of novel experimental and theoretical results on application issues. As an example consequences of the so called reverse melting or the reverse vitrification on model of the mantle of the Earth or on some issue associated with the food conservation can serve.

Following these issues, the post-ESF EW special volume of the Journal of Physics: Condensed Matter "*Glassy Liquids under Pressure*" may appear to be an important reference for research society involved in studies on the vitrification phenomenon

#### **3.2 Establishing new Pan-European Network and Projects**

This ESF EW was also planned as an intellectual agenda to form a basis for arranging Pan-European, Transnational, Network and Projects.

The first stage of this target was reached just after this ESF EW, namely: For the call for the ESF Networking Programmes with 30<sup>th</sup> Oct., 2007 deadline the application entitled "*Glassy Liquids under Pressure*" was submitted. It was arranged by A. Drozd-Rzoska, J. Ll. Tamarit and S. J. Rzoska, basing on the agreement at the ESF EW "*Glassy Liquids under Pressure: Fundamentals and Applications*". Its reference number in European Science Foundation: "2662".

The next Network, within FP7 focusing on nanoparticles, complex liquids and exogenic impacts is under preparation

Several bilateral cooperation links were established during the Workshop.

### **3.3 Post ESF EW Publicity important for the research&application output of the ESF EW:**

- (a) A unique publicity, important for the glass transition focused researchers in general, is the mentioned special issue of the Journal of Physics: Condensed Matter "*Glassy Liquids under Pressure*". It will contain articles related to all lectures presented at the meeting, up-to-dated due to the brainstorming discussion at the ESF EW. The ESF will be recalled at the cover of this issue and in the introductory article. The order of articles will be arranged by convenors, to create a kind of a handbook in this challenging field. Each author-participant (of the ESF EW) will obtain a free copy of this special issue. We would like to recall the commonly recognized prestigious position of the Journal of Physics: Condensed Matter.
- (b) An article the "*Gazeta Uniwersytecka*" – the monthly journal of the Silesian University society describing the meeting "The mystery of the transition to the glassy state" (english translation) was prepared by Aleksandra Drozd-Rzoska. This paper, broadly written by the Silesian University students and employees, present the general problem of the glass transition as well impressive possibilities open due to the application of pressures. It also contains basic facts about the ESF, its programmes as well as about ESF Exploratory Workshops scheme. All this was illustrated by photos of (i) Josep Ll. Tamarit speaking about the ESF at the introductory lecture (ii) Participants of the ESF EW during one of lectures (iii) the general ESF EW photo, in the garden of "Hotel Jaskolka", the conference loci. This article may be important for students in Poland.

## 4. Final Programme

### Wednesday 10 October 2007

Afternoon	<i>Arrival &amp; Registration:</i> Institute of Physics Silesian University 4 Uniwersytecka, str. 40-007Katowice
20.45	<i>Departure to <b>Ustron</b> (conference site) by bus</i>
22.30	<i>Dinner in Hotel Jaskółka, the ESF EW loci.</i>

### Thursday 11 October 2007

09.00	<b>Meeting introduction by the convenors</b>
09.15	<b>Presentation of the European Science Foundation (ESF) by Jose Ll. Tamarit (Spain)- the co-convenor</b>
<b><u>PANEL I :</u></b>	<b>Glassy Liquids under Pressure: General Issues</b>
09.30 – 11.00	<b>SESSION 1</b>  <b>Kia L. Ngai</b> (USA/Italy): "Significant Impact of Pressure Studies on Fundamental Understanding of Glass Transition: Theory and Experiments".  <b>Vadim Brazhkin</b> (Russia): "Puzzling Behaviour of Liquids at multi-GPa Pressure Range: Recent Examples".  <b>Isak Avramov</b> , (Bulgaria): "Pressure Dependence of Viscosity or is the Earth Mantle a Glass?".
11.00 – 12.00	<i>Coffee Break &amp; Discussion</i>
12.00 – 13.00	<b>SESSION 2</b>  <b>Thomas Voigtmann</b> (U.K.): "Glasses under High Pressure a Mode-Coupling Perspective".  <b>Marian Paluch</b> (Poland): "Thermodynamical Scaling in Glass-Forming Liquids".
13.00 - 15.30	<i>Lunch</i>
15.30 – 17.00	<b>SESSION 3</b>  <b>Ulrich Buchenau</b> (Germany): "Dielectric Relaxation in Molecular Glasses".  <b>Gabriel Cuello</b> (France): "Structure of Amorphous Materials : Neutron diffraction".  <b>Alberto Rivera</b> (Spain): "Electric Response of Room Temperature Ionic Liquids under Pressure".
17.00 - 17.30	<i>Coffee Break &amp; Discussion</i>

17.30 – 18.30

#### **SESSION 4**

**Simone Capaccioli** (Italy): "Interdependence of Primary and Secondary Relaxations under Pressure and Temperature Variations in Glass Forming Systems".

**Sylwester J. Rzoska** (Poland): "Direct Insight into Heterogeneous Dynamics from the Nonlinear Dielectric Spectroscopy".

**Workshop Dinner & Evening discussions**

### **Friday 12 October 2007**

#### **PANEL II: Liquid-Liquid Transition, Pressurization & the Glass Transition Puzzle**

09.00 – 10.30

#### **SESSION 5**

**Mark Wilson** (U.K.): "Evidence for Polyamorphism from Computer Simulation".

**Martin Wilding** (U.K.): "Fragility, Polyamorphism and Amorphous Structure: Neutron Diffraction studies of Silicate Glasses at High Pressure".

**Jeppe Dyre** (Denmark): "One or More Order Parameters: The High-Pressure Perspective".

10.30 - 11.00

*Coffee Break & Discussion*

11.00 – 12.30

#### **SESSION 6**

**Marie-Claire Bellisant-Funel** (France): "Influence of Pressure on Water-Biomolecules Systems. Applications for Food Industry".

**Victor Teboul** (France): "Dynamical Heterogeneity in Supercooled Water" the Effect of Confinement and Pressure".

**Giancarlo Franzese** (Spain): "Dynamics of Supercooled Liquid Water: Novel Pressure Effects".

12.30 - 14.00

*Lunch*

14.00 – 15.00

#### **SESSION 7**

**Ove Andersson** (Sweden): "Production and Investigations of Amorphous States by Means of High Pressure".

**Juergen Horbach** (Germany): "Amorphous Silica under Pressure: A Computer Simulation Study".

15.30 - 15.30

**Coffee Break & Discussion**

15.30 – 16.30

#### **SESSION 8**

**Victor Mazur** (Ukraine): "Two-Fluid Model of Glassy Liquids".

**Jerzy Ziolo** (Poland): "Liquid-Liquid Transition in a Simple, One Component and Non-Mesogenic Liquid".

16.30

### **Dinner & Discussion**

#### **Social Programme: "Highlanders' evening"**

Sponsored by Universitat Politècnica de Catalunya & Silesian University.

## **Saturday 13 October 2007**

### **PANEL III : Vitrification under Pressure: New Opportunities**

8.30 – 10.00

#### **SESSION 9**

**Attila Imre** (Hungary): "Fragility of Liquids, Solids and Glasses".

**Josep Ll. Tamarit** (Spain): "High Properties Inferred from Normal-Pressure Properties".

**Phil Salmon** (U.K.): "Structure of Tetrahedral Glass Forming Systems: from Ambient to High Pressures".

10.30

#### **Excursion to Koniakow**

*(– a small and very picturesque village in Beskidy Mountains). This included a visit in a 600 years old church made from wood and subsequently the visit in a traditional highlander house from the XIXth century with presentation of some old traditions.*

13.30

**Lunch** in Karczma (in Polish this means "very traditional restaurant") "Ochodzita" in Koniakow

15.00 – 16.00

#### **SESSION 10**

**Jan Thoen** (Belgium): "Thermal and Dielectric Spectroscopy of Glass Forming Liquids and Confinement Effects".

**Samo Kralj** (Slovenia): "Influence of Nano-Particles on Phase and Structural Properties of Liquid Crystals".

16.00 - 17.00

#### **Coffee Break & Discussion**

17.00 - 18.00

#### **SESSION 11**

**George Floudas** (Greece): "Glass Transition in Discotic Liquid Crystals - Effects of Pressure".

**Aleksandra Drozd-Rzoska** (Poland): "Glassy Dynamics in Rod-Like Liquid Crystalline Compounds".

#### **Dinner**

#### **SESSION 12:**

#### **Closing Brainstorming Discussion: "Pressure Related Studies: The Way for Solving the Glass Transitions Puzzles?"**

***The purpose of this session was also to explore means of setting up***

The discussion continued till midnight. The catering with coffee, tea, refreshments, small sandwiches and cakes was available permanently.

## Sunday 14 October 2007

08.00-9.00

### **Breakfast**

### **Departure**

(Travel time from Ustron to Katowice: ca. 90 min.)

*The bus first arrived to the Katowice-Pyrzowice airport, next to Hotel Uniwersytecki in Katowice and finally to the Institute of Physics, Silesian University in the clear centre of Katowice.*

*There were very vivid discussions during the ESF EW, extending even to midnight. Following this at the closing discussion all participants agreed to published results presented at the ESF EW in the special volume of the Journal of Physics: Condensed Matter (JPCM) – the possibility arranged by Aleksandra Drozd-Rzoska in negotiations with Robert Palmer, the chief editor of JPCM.*

*At the closing discussion the common agreement for arranging pan-European Networks was established. Such application, for the ESF Networking Programme, was submitted already for the call finished at 30<sup>th</sup> Oct. 2007, by A. Drozd-Rzoska, J. Ll. Tamarit and S. J. Rzoska, in cooperation with the majority of ESF EW participants.*



## 4. Statistical Information on Participants

### Nationalities:

Belgium	1
Bulgaria	1
Denmark	1
France	3
Germany	3
Greece	1
Hungary	1
Italy	2
Poland	4
Slovenia	1
Spain	4
Sweden	1
Russia	1
UK	2
Ukraine	1

### **TOTAL: 27 persons**

There was no ESF representative.

### Gender Repartition:

Female participants: 2

Male participants: 25

A nice "age" equilibrium was also reached. Data of all participants, including the age were introduced into the ESF data base before the meeting.

## 5. List of participants (*including convenors*)

<b>1. Aleksandra DROZD-RZOSKA (convenor)</b> Institute of Physics, Silesian University ul. Uniwersytecka 4, 40-007 Katowice, <b>POLAND</b> e-mail: <a href="mailto:rzoska@us.edu.pl">rzoska@us.edu.pl</a> tel: +48 32 3591628 mobile: +48 660 43 85 96	<b>2. Josep Lluís TAMARIT (co-convenor)</b> Polytechnica de Catalunya (ETSEIB) Diagonal 647 080 208 Barcelona, Catalonia, <b>SPAIN</b> e-mail: <a href="mailto:jose.luis.tamarit@upc.es">jose.luis.tamarit@upc.es</a> tel: +34 93 401 65 64
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*There were also two technicians, not counted among the participants.*

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