

Glass transition and relaxation behavior of water and aqueous solutions

Jan Swenson

Department of Applied Physics, Chalmers University of Technology
SE-412 96 Göteborg, Sweden

Email address: jan.swenson@chalmers.se

This presentation focuses on two topics; the glass transition temperature of water and an ultraslow (i.e. slower than the viscosity related α -relaxation) relaxation process in water and aqueous solutions. In the case of the ultraslow Debye-like relaxation it is well known that such a process exists in monoalcohols [1], although its origin is still not clear. For monoalcohols this slow Debye-like relaxation is 2-3 orders of magnitude slower than the viscosity related α -relaxation, and it is also much more intense [1]. Here we show that a similar Debye-like process exists also in other hydrogen bonded liquids, such as water and aqueous solutions, although its intensity is substantially weaker than in the monoalcohols, and also a few more orders of magnitude slower than the α -relaxation [2,3]. Whether this weak and ultraslow process in a wide range of hydrogen bonded liquids has the same physical origin as the well-known Debye-like relaxation in monoalcohols remains to be elucidated.

Regarding the glass transition of water many different scenarios have been discussed in recent years, although the most accepted glass transition temperature of bulk water is still the 136 K, as proposed by Johari *et al.* [4]. Here we try to understand the glass transition related dynamical properties of supercooled bulk water from experimental results on interfacial water. We propose [5] that the commonly accepted glass transition temperature of bulk water at 136 K is not a true glass transition, but rather due to the freezing in of a local secondary β -relaxation. The true glass transition should instead be located close to the critical temperature $T_s \approx 228$ K when the build-up of an ice-like tetrahedral network structure is completed. The proposed interpretation is simple and able to explain many of the peculiar properties of supercooled water. For instance, it explains (a) the weakness of the calorimetric feature at 136 K, (b) why bulk water crystallizes immediately slightly above 228 K, (c) the unusual density behavior below 277 K, and (d) the similarities to ice at low temperatures. Furthermore, the model is closest to the findings for confined water and aqueous solutions, and no speculative liquid-liquid transition or fragile-to-strong transition is needed to explain the properties of supercooled and glassy water.

References

- [1] L. M. Wang and R. Richert, *J. Chem. Phys.* 121, 11170 (2004).
- [2] R. Bergman, H. Jansson, and J. Swenson, *J. Chem. Phys.* 132, 044504 (2010).
- [3] H. Jansson, R. Berman, and J. Swenson, *Phys. Rev. Lett.* 104, 017802 (2010).
- [4] G. P. Johari, A. Hallbrucker and E. Mayer, *Nature (London)* 330, 552 (1987).
- [5] J. Swenson and J. Teixeira, *J. Chem. Phys.* 132, 014508 (2010).