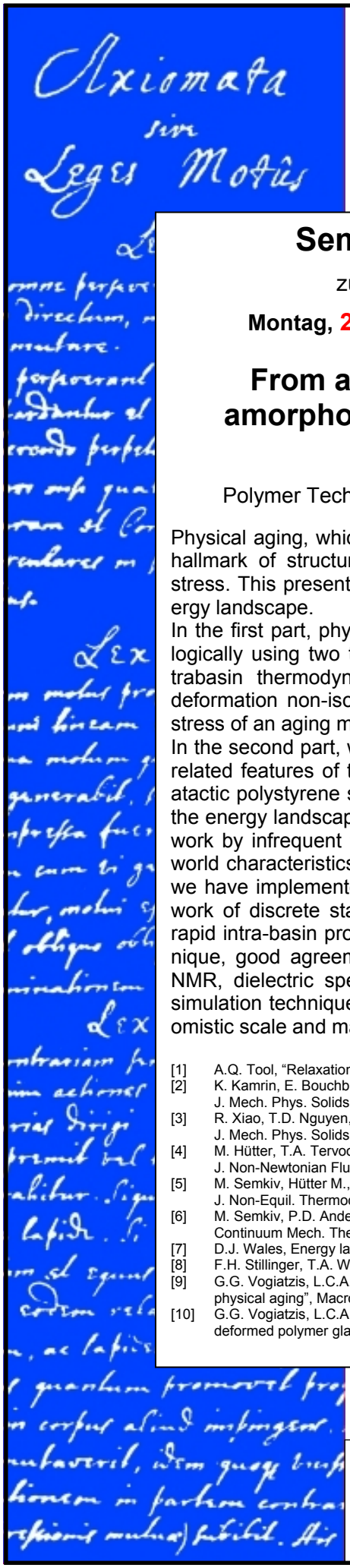

FRIEDRICH-ALEXANDER UNIVERSITÄT ERLANGEN-NÜRNBERG
TECHNISCHE FAKULTÄT

Seminar über Fragen der Mechanik

zu folgendem Vortrag wird herzlich eingeladen

Montag, 27.04.2020, 14:00 Uhr, Egerlandstr. 5, Raum 0.044

From atoms to the continuum mechanics of amorphous solids: energy-landscape approach

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Physical aging, which originates from slow ongoing changes in the microstructure, is a hallmark of structural glasses, and affects many physical properties, e.g. the yield stress. This presentation addresses the modeling of such materials in terms of the energy landscape.

In the first part, physical aging and mechanical rejuvenation are modeled phenomenologically using two temperatures, characterizing phenomenologically the inter- and intrabasin thermodynamics [1-3], respectively. Doing so in combination with finite-deformation non-isothermal mechanics [4] also leads to the conclusion [5,6] that the stress of an aging material is in general hypoelastic, rather than hyperelastic.

In the second part, we proceed to unraveling the atomistic origins of physical aging and related features of the glass. The results of a Molecular Dynamics (MD) simulation of atactic polystyrene show that, in the course of time, the system visits several basins in the energy landscape, which are envisioned as discrete states [7,8] connected to a network by infrequent transitions. It is shown that this network has scale-free and small-world characteristics [9]. In order to overcome time-scale limitations in MD simulations, we have implemented a computational technique that focusses on generating the network of discrete states connected by infrequent transitions over saddle points, while rapid intra-basin properties are captured by the basin free energy [10]. Using this technique, good agreement is obtained with experimental data on infrared-spectroscopy, NMR, dielectric spectroscopy, and mechanical properties. The major benefit of the simulation technique is that it allows to make a direct link between the dynamics on atomistic scale and macroscopic observations.

[1] A.Q. Tool, “Relaxation of stresses in annealing glass”, J. Res. Natl. Bur. Stand.(US), 34, 199-211 (1945)
[2] K. Kamrin, E. Bouchbinder, “Two-temperature continuum thermomechanics of deforming amorphous solids”, J. Mech. Phys. Solids, 73, 269-288 (2014).
[3] R. Xiao, T.D. Nguyen, “An effective temperature theory for the nonequilibrium behavior of amorphous polymers”, J. Mech. Phys. Solids, 82, 62-81 (2015).
[4] M. Hütter, T.A. Tervoort, “Thermodynamic considerations on non-isothermal finite anisotropic elasto-viscoplasticity”, J. Non-Newtonian Fluid Mech., 152, 53-65 (2008).
[5] M. Semkiv, Hütter M., “Modeling aging and mechanical rejuvenation of amorphous solids”, J. Non-Equil. Thermodyn., 41, 79-88 (2016).
[6] M. Semkiv, P.D. Anderson, M. Hütter, “Two-subsystem thermodynamics for the mechanics of aging amorphous solids”, Continuum Mech. Thermodyn., 29, 647-663 (2017).
[7] D.J. Wales, Energy landscapes, Cambridge University Press (2003).
[8] F.H. Stillinger, T.A. Weber, “Hidden structure in liquids”, Phys. Rev. A, 25, 978-989 (1982).
[9] G.G. Vogiatzis, L.C.A. van Breemen, M. Hütter, “Network topology of the states probed by a glassy specimen during physical aging”, Macromol. Theory Simul., 28, 1900036 (2019).
[10] G.G. Vogiatzis, L.C.A. van Breemen, D.N. Theodorou, M. Hütter, “Free energy calculations by molecular simulations of deformed polymer glasses”, Comput. Phys. Commun., (in press) (2019). https://doi.org/10.1016/j.cpc.2019.107008

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