I18 - Wed 13:50-14:20   **Glass Transition 2**   Großer Saal / Great Hall

Two glass transitions in liquid metals. Molecular modelling.

Genri E. Norman, Vasily V. Pisarev

Joint Institute for High Temperatures of RAS, Moscow, Russia

Glass transition in metals is investigated by the molecular dynamics (MD) method on the example of liquid aluminum. The transition temperature is found using several criteria based melt microstructure, diffusivity and specific heat. The dependence of glass transition temperature on cooling rate is found for each of these criteria. Two characteristic temperature ranges are found. Changes in microstructure and the self-diffusion activation energy occur in the range 820-880 K, while heat capacity changes are observed in the range 500-600 K [1]. The dependence of the "calorimetric" glass transition on cooling rate follows Bartenev's formula, while "structural" glass transition behaves according to the Vogel-Fulcher-Tammann relaxation law, which has also been found in polymer glasses [2].

Viscosity calculations are performed to find out the temperature which corresponds to the solidification of the melt [3]. Viscosity is calculated using the Green-Kubo relation which is based on the integration of shear stress autocorrelation function (SACF). The power-law decay ($t^{-\alpha}$) is found for the SACF tails, and the exponent α dependence on temperature is obtained. α=3/2 at high temperatures and diminishes at cooling. In the range 800-900 K, α starts to deviate from the high-temperature limit, and the value α=1 is crossed in the range 550-600 K. Therefore, the integral of the SACF diverges below 550 K, and the viscosity becomes infinite. Thus, both glass transition intervals are explained by the changes of a single parameter — SACF tail exponent.

References:
[1] L.N. Kolotova, G.E. Norman, and V.V. Pisarev, J. Non-Cryst. Solids **429**, 98 (2015).
[2] J.W. Schmelzer, and T.V. Tropin, J. Chem. Phys. **138**, 034507 (2013).
[3] E.M. Kirova, and G.E. Norman, J. Phys.: Conf. Ser. **653**, 012106 (2015).

C54 - Wed 14:20-14:40   **Glass Transition 2**   Großer Saal / Great Hall

Relaxation dynamics of metallic systems in the liquid/glass transition region.

Chaoren Liu[1], Eloi Pineda[1], Daniel Crespo[1]

[1] Universitat Politècnica de Catalunya – BarcelonaTech, Department of Physics, Castelldefels, Spain

The liquid/glass transition is controlled by structural dynamics with characteristic times changing from 10^{-2} to 10^{4} s within the $0.9T_g$-$1.1T_g$ temperature range. In metallic systems this slow dynamics is usually probed by means of calorimetric, mechanical spectroscopy and quasi-static stress relaxation measurements[1][2]. However, the accessible time window is usually restricted to 10^{-1}-10^{2} s due to limitations of the experimental techniques, instability against crystallization, physical aging or sample geometry restrictions in the case of low-GFA alloys. For instance, the characterization of the main α-relaxation in the sub-T_g region is usually estimated indirectly, assuming the response of the material maintains similarity along the whole temperature region and applying the time-temperature-superposition principle[3]. This similarity, however, is not fulfilled if aging, secondary relaxations or nonlinear response are present in the system and very few studies have been devoted to fully characterize the extremely slow α-relaxation in the sub-T_g region.

In this work we present experimental characterization and modeling of the relaxation spectrum of Mg-Cu-Y, Cu-Zr-Al, Pd-based and Fe-based metallic glass-forming alloys in the $0.9T_g$-$1.1T_g$ range. After subtracting the secondary relaxation contribution, minimizing the effect of aging and normalizing by T_g, an interesting result is that the sub-T_g α-relaxation shows common temperature and frequency dependences, while the liquid state above T_g shows different temperature behaviors as expected by the different liquid fragilities of the studied alloys. The similarity of the dynamics below T_g indicates that the nature of the microscopic mechanisms involved in the full macroscopic relaxation is similar in all metallic systems once arrested in an isoconfigurational state. The different degrees of inhomogeneity frozen in in the glassy structure, which are also known to be related to the different liquid fragilities, affect the intensity of secondary relaxations and other features of the relaxation spectrum but they seem to have little influence on the main relaxation process.

References:
[1]   C. Liu, E. Pineda and D. Crespo, J. Alloys Compd. **Vol. 643**, S17–S21 (2015).
[2]   C. Liu, E. Pineda and D. Crespo, Metals **Vol. 5**, 1073–1111 (2015).
[3]   C. Liu, E. Pineda, J. Qiao, D. Crespo, J. Phys. Chem. B. Vol. 120, 2838–44 (2016).