

CPP 47: P12: Glasses and Glass Transition

Time: Wednesday 10:00–13:00

Location: Poster A

CPP 47.1 Wed 10:00 Poster A

The effect of finite temperatures on jammed packings — ●CLEMENS BUSS¹, CLAUS HEUSSINGER², and OSKAR HALLATSCHKEK³ — ¹Max-Planck-Institut für Dynamik und Selbstorganisation (MPIDS) Bunsenstrasse 10, D-37073 Göttingen — ²Institute for theoretical Physics University of Goettingen Friedrich Hund Platz 1 37077 Goettingen — ³Department of Physics University of California 366 LeConte Hall MC 7300 Berkeley, CA, 94720-7300

We study the effect of finite temperatures on jammed packings. The packings are obtained through a standard energy minimization protocol. We then study their thermodynamic properties by simulating them at finite temperature through a Monte Carlo Metropolis scheme. Based on our simulation model, we can determine mechanical and thermodynamical properties and how they behave for different temperatures, external pressure and coordination numbers. The quantities we measure comprise the thermal expansion, bulk and shear modulus as well as the phase diagram. Together with theoretical arguments we can explain crucial parts of the results and the scaling behaviour. In the last step we connect those findings to real materials such as silica glass.

CPP 47.2 Wed 10:00 Poster A

Molecular dynamics of polymethylphenylsiloxane under 1-D and 2-D geometrical confinement- a comparison — ●WYCLIFFE K. KIPNUSU¹, MOHAMED ELSAYED², EMMANUEL U. MAPESA¹, REINHARD KRAUSE-REHBERG², and FRIEDRICH KREMER¹ — ¹Institute of Experimental physics I, Linnstr.5, 04103, Leipzig — ²Martin-Luther-Universität Halle-Wittenberg)

Molecular dynamics of polymethylphenylsiloxane (PMPS) in 1-D (thin films) and 2-D (silica nanopores with pores sizes of 8, 6, and 4 nm) geometrical constraints are studied by broadband dielectric spectroscopy (BDS) while Positron annihilation lifetime spectroscopy (PALS) is employed to probe the free volume in the bulk PMPS and under 2D confinement. The glass transition temperature (T_g) of thin films down to 5 nm remained bulk-like but the T_g decreases with the reduction of pores sizes for 2-D confinement where additional interfacial relaxation process is observed. This process is removed after silanization of the pores. The change in T_g is attributed to the reduction of density of bulk-like molecules at the center of the pores. This is proven by the PALS results which indicate that the average free volume increases with decreasing pore sizes. This shows how the dimensionality of confinement and packing density of the molecules impacts on the molecular dynamics.

CPP 47.3 Wed 10:00 Poster A

Glass transition coopeativity from broad band heat capacity spectroscopy — ●YEONG ZEN CHUA¹, GUNNAR SCHULZ¹, EVGENI SHOIFET¹, HEIKO HUTH¹, REINER ZORN², JÜRN W.P. SCHMELZER¹, and CHRISTOPH SCHICK¹ — ¹Institute of Physics, University of Ro-

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Molecular dynamics is often studied by broad band dielectric spectroscopy (BDS) because of the wide dynamic range available and the large number of processes resulting in electrical dipole fluctuation and with that in a dielectrically detectable relaxation process. Calorimetry on the other hand is an effective analytical tool to characterize phase and glass transitions by its signatures in heat capacity. In the linear response scheme, heat capacity is considered as entropy compliance. Consequently, only processes significantly contributing to entropy fluctuations appear in calorimetric curves. The glass relaxation is prominent example for such a process. Here we present complex heat capacity at the dynamic glass transition (segmental relaxation) of polystyrene (PS) and poly(methyl methacrylate) (PMMA) in a dynamic range of 11 orders of magnitude, which is comparable to BDS. As one of the results, we determine the temperature dependence of the characteristic length of the corresponding fluctuations. The characteristic length decreases from about 4 nm to about 0.7 nm in the temperature range from 370 K to 500 K. This proves an estimate for possible confinement effects on the segmental relaxation, which is different from vitrification as discussed by Cangialosi et al.

CPP 47.4 Wed 10:00 Poster A

Glass transition coopeativity from broad band heat capacity spectroscopy — ●YEONG ZEN CHUA¹, GUNNAR SCHULZ¹, EVGENI SHOIFET¹, HEIKO HUTH¹, REINER ZORN², JÜRN W.P. SCHMELZER¹, and CHRISTOPH SCHICK¹ — ¹Institute of Physics, University of Rostock, Wismarsche Str. 43-45, 18051 Rostock, Germany — ²Juelich Centre for Neutron Science, 52425, Juelich, Germany

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