



Contribution ID: 10

Type: **Invited talk**

Inelastic and quasielastic neutron scattering on microporous polymer membranes for green separation processes

Wednesday, 1 June 2022 09:00 (35 minutes)

Inelastic and quasielastic neutron scattering on microporous polymer membranes for green separation processes

Andreas SCHÖNHALS¹, Paulina SZYMONIAK¹, Reiner ZORN², Martin BÖHNING¹

¹Bundesanstalt für Materialforschung und -prüfung, Unter den Eichen 87, 12489 Berlin, Germany

²Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science (JCNS-1) and Institute for Biological Information Processing (IBI-8), 52425 Jülich, Germany

Polymers with intrinsic microporosity are promising candidates for the active separation layer in gas separation membranes. These polymers are characterized by a high permeability and reasonable permselectivity. The latter point is somehow surprising because for microporous systems a more Knudsen-like diffusion is expected than a size dependent temperature activated sieving process. It was argued in the framework of a random gate model that molecular fluctuations on a time scale from ps to ns are responsible for the permselectivity [1].

Here a series of microporous polynorbornenes with bulky Si side groups and a rigid backbone are considered which have different microporosity characterized by BET surface area values.

First inelastic time-of-flight neutron scattering measurements were carried out to investigate the low frequency density of state (VDOS). The measured data show the characteristic low frequency excess contribution to the VDOS above the Debye sound wave level, generally known as the Boson peak in glass-forming materials. It was found the maximum position of the Boson peak correlates with the BET surface area value [2].

For two selected comparable polynorbornenes elastic scans as well as QENS measurements by a combination of neutron time-of-flight and backscattering are carried out [3]. A low temperature relaxation process was found for both polymers. This process was assigned to the methyl group rotation. It was analysed in terms of a jump diffusion in a three-fold potential. The analysis of the dependence of the elastic incoherent structure factor on the scattering vector yields the number of methyl groups which might be immobilized.

[1] R. Inoue, T. Kanaya, T. Masuda, K. Nishida, O. Yamamuro *Macromolecules* 45, 6008 (2012)

[2] R. Zorn, P. Szymoniak, M. A. Kolmangadi, A. Wolf, D. Alentiev, M. Bermeshev, M. Böhning, A. Schönhals *Physical Chemistry Chemical Physics* 22, 18381 (2020)

[3] A. Schönhals, P. Szymoniak, M. A. Kolmangadi, M. Böhning, M., Zamponi, B. Frick, M. Appel, G. Günther, M. Russina, D. Alentiev, M. Bermeshev, R. Zorn, R. *Journal of Membrane Science* 642 119972 (2022)

E-mail for corresponding author: andreas.schoenhals@bam.de

Presenter: Prof. SCHÖNHALS, Andreas (BAM Berlin)

Session Classification: Wednesday morning

Track Classification: Main