Extraction of Mechanical Parameters via MD Simulation: Application to Polyimides

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Introduction

Determining physical properties from simulations is an important task for every simulation engineer. Physical properties are often used to verify the representation of the real behavior by the simulation. By representing physical properties that can easily be determined with experiments it is possible to assume an accurate determination of properties of interest. In former works the glass-transition temperature as well as the density were already determined.

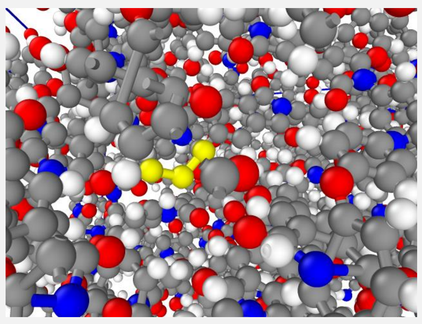

Fig. 1: Sulfur dioxide molecule in PMDA-ODA polyimide matrix.

In this work the Young's modulus and the Poisson's ratio were determined to verify the accurate description of the system with the used force-field. Additionally, the density as well as the glass-transition temperature were already determined and compared with literature data.

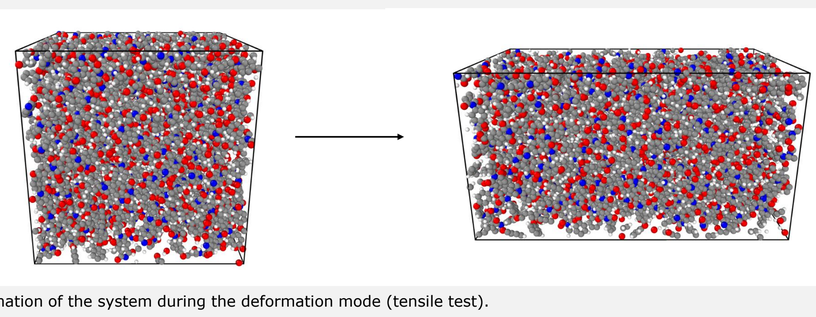

Fig. 2: Deformation of the system during the deformation mode (tensile test).

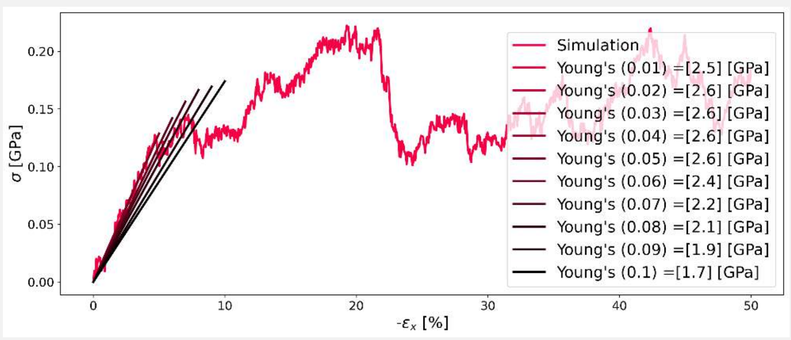

Fig. 3: Stress-strain diagram of system C during the slow deformation mode simulation.

Methodology

The first way to determine both Young's modulus and Poisson's ratio was the simulation of the well-established tensile test (Fig. 4) that is used in conventional material testing. In this simulation setup the system gets stretched or compressed uniaxial (e.g. in x-axis) with a given deformation rate. To allow for an objective determination of the Young's modulus the anisotropy Γ (Fig. 5) was introduced to describe the isotropy of the system.

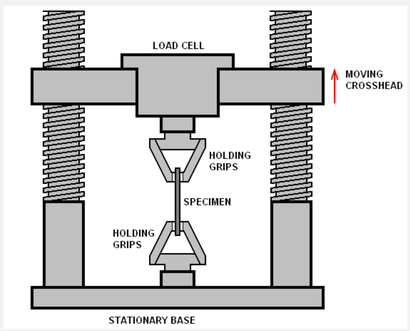

Fig. 4: Tensile test setup[1].

The second way was the so-called relaxation mode. In this case the system gets deformed immediately after the relaxation by a pre-defined percentage in 1 direction. In the second step the system is allowed to relax, the tension and deformation are measured, which allows to calculate both Young's modulus and Poisson's ratio (Fig. 6).

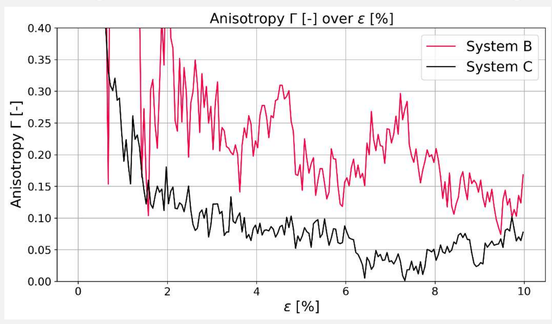

Fig. 5: Anisotropy Γ of system B and C over the deformation.

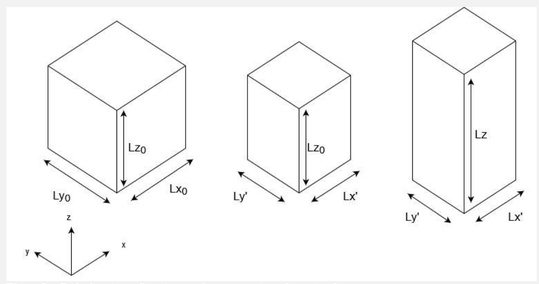

Fig. 6: Prinicple of relaxation mode simulation.

[1] http://www.engineeringarchives.com/les_mom_tensiletest.html

Results

The results were compared for different temperatures, different pressures, two distinct system sizes and two different determination modes. In the case of the deformation mode, i.e. the tensile test, a range for both the R^2 of the linear representation of the results and the anisotropy were defined to allow for an objective determination of the results. The table is shown in Fig. 7.

log_C1_SD_C-1e-6 (1atm)								
	X	Y	Z	anisotropy	X	Y	Z	
ε	R^2			Γ	E [Gpa]			average
1%	0.7946	0.1103	0.8517	0.2004	2.15	4.14	2.25	2.847
2%	0.9129	0.8484	0.9658	0.1931	2.16	3.4	2.28	2.613
3%	0.9392	0.9277	0.9790	0.1597	2.23	3.11	2.37	2.570
4%	**0.9640**	**0.9349**	**0.9828**	**0.0860**	**2.22**	**2.89**	**2.27**	**2.460**
5%	0.9758	0.9460	0.9787	0.1273	2.17	2.75	2.18	2.367
6%	**0.9744**	**0.9519**	**0.9840**	**0.0713**	**2.09**	**2.64**	**2.14**	**2.290**
7%	**0.9748**	**0.9389**	**0.9755**	**0.0709**	**2.03**	**2.51**	**2.06**	**2.200**
8%	**0.9749**	**0.9135**	**0.9592**	**0.0692**	**1.98**	**2.38**	**1.97**	**2.110**
9%	**0.9692**	**0.8858**	**0.9384**	**0.0533**	**1.92**	**2.25**	**1.88**	**2.017**
10%	0.9522	0.8299	0.8856	0.0858	1.84	2.12	1.76	1.907

Fig. 7: Result matrix of the slow deformation mode simulation of system C for compression at 1e-6 deformation rate.

In general, it can be said that the relaxation mode is pressure dependent, that the bigger system C gives better results for both modes and both Young's modulus and Poisson's ratio in comparison to literature data.

Outlook / Next Steps

In the next step focus will be on the determination of transport properties of corrosive gases and ions within the polyimide matrix. For the determination of adsorption and diffusion a free-standing membrane was already prepared (Fig. 8). With this setup it will be possible to simulate concentration gradients and an electric field that pushes the ions through the polymer.

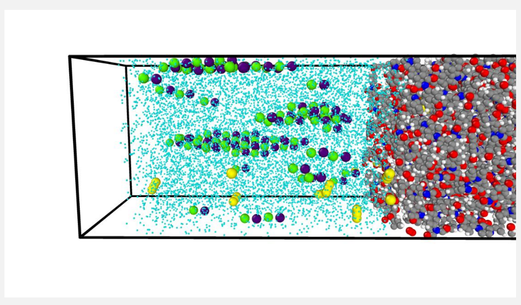

Fig. 8: Chamber of water with K+ and Cl- ions and half of the free-standing membrane.

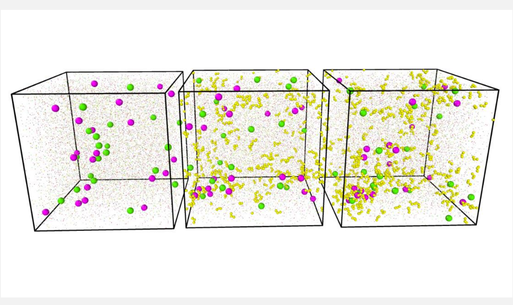

Fig. 9: Polymer bulk with different water content (from left to right: 0wt%, 3wt%, 10wt%) and dissolved K+ and Cl- ions.

Additionally, simulations with different water contents in the bulk are conducted to determine the bulk self-diffusion coefficient of the ions (Fig. 9) .

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