Supporting Information

Structure and Properties of High and Low Free Volume Polymers Studied by Molecular Dynamics Simulation

Mikhail Mazo, Nikolay Balabaev, Alexandre Alentiev, Ivan Strelnikov and Yury Yampolskii

I. Correlation between the number of chain ends and polymer density

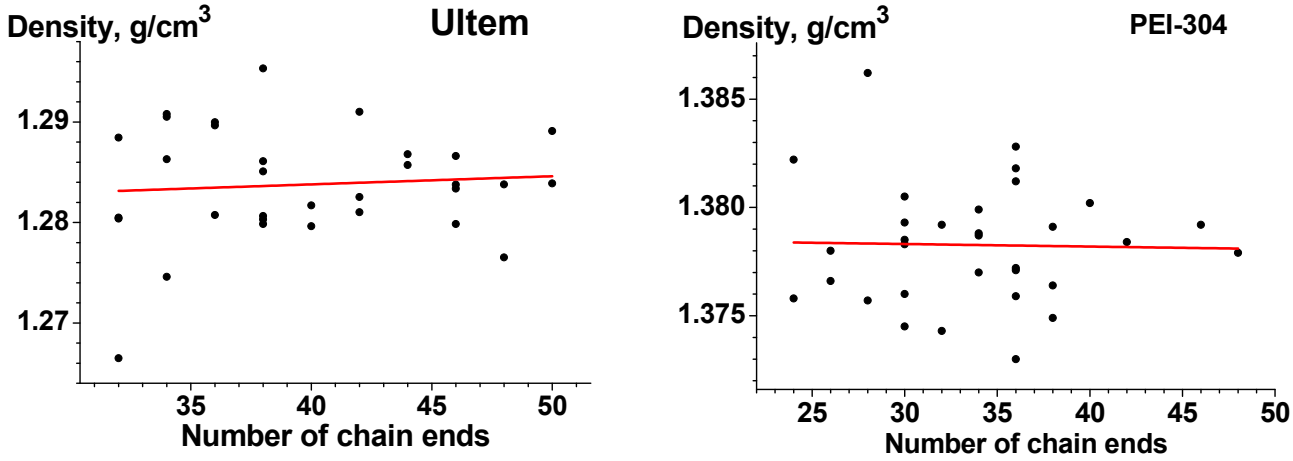

Figure S1. Dependence of density on the number of chain ends in samples. Red lines show the best fit. Pearson correlation coefficients are 0.08 and –0.02 for ULTEM and PEI-304 relatively.

II. On the dependence between the ends of chains (L, Å) versus the number of repeat units in the chains (N).

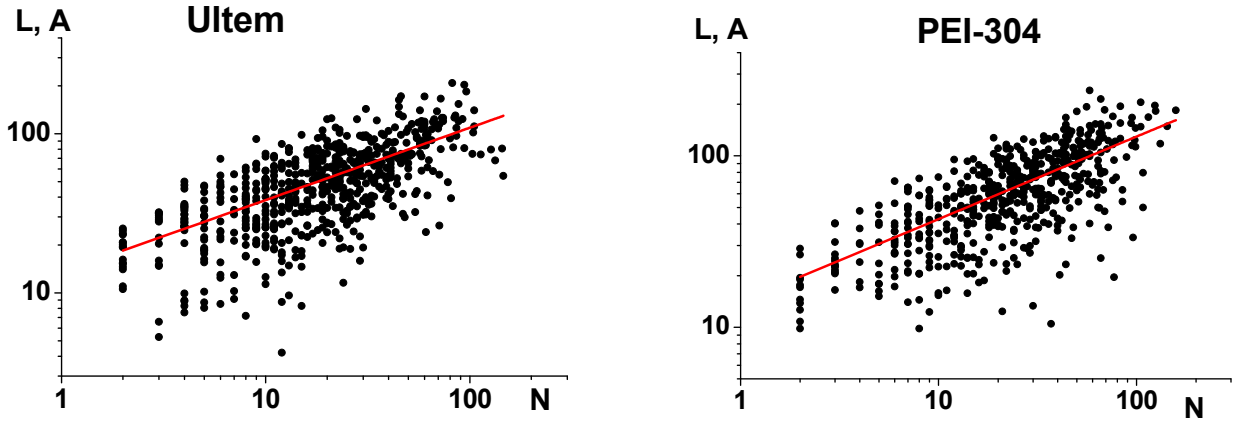

Figure S2. Dependence of the distance between the ends of chains L (Å) and the number of repeat units in them N. For every polymer all the chains from 32 samples are considered. The red lines are the linear regression, their parameters are given in Table S1.

Table S1. Parameters of linear regression from figure S2 ($\log_{10}L=A+B\ \log_{10}N$)

	A	B
Ultem	13.5 ±1.0	0.45 ±0.02
PEI-304	14.1 ±1.2	0.48 ±0.02

III. Visualization of free volume

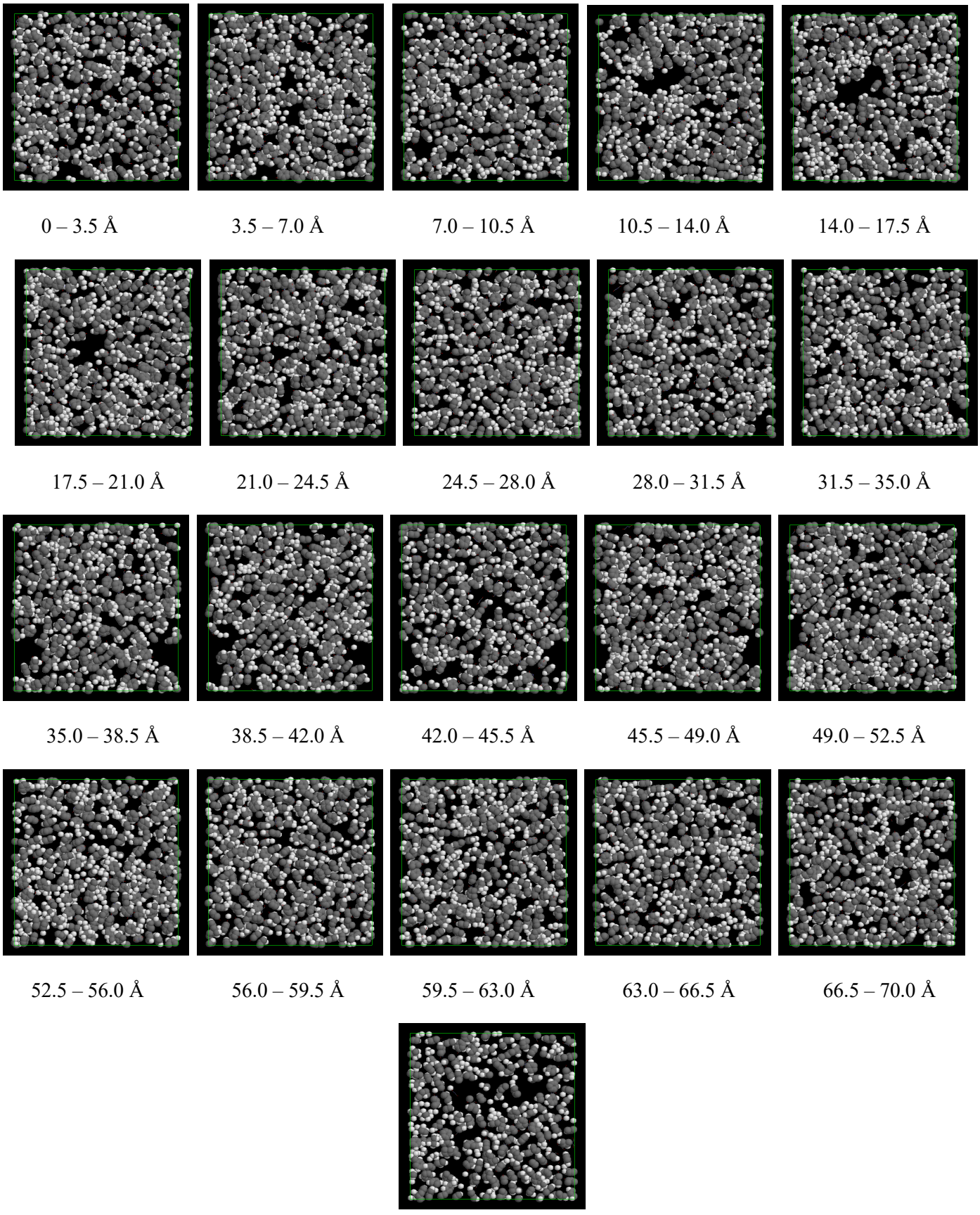

Figure S3. Visualization of free volume of Ultem model. ρ= 1.279 g/cm^3, cross sections are shown through 3.5 A along the Z axis.

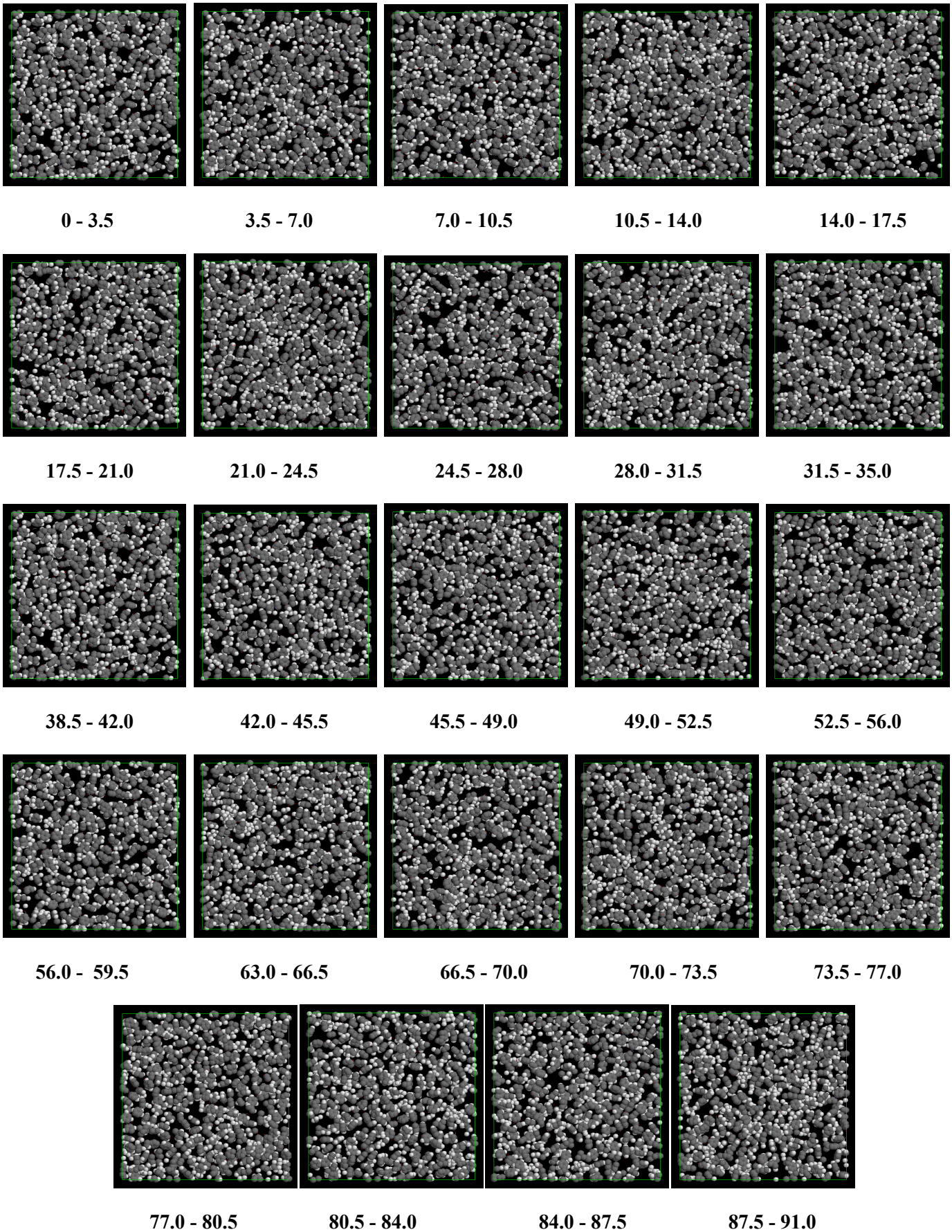

Figure S4. Visualization of free volume of PEI-304 model. ρ= 1.376 g/cm^3, cross sections are shown through 3.5 A along the Z axis.