View metadata, citation and similar papers at core.ac.uk

brought to you by CORE

provided by Online Research Database In Technology

Developing a Macroscopic Mechanistic Model for Low Molecular Weight Diffusion through Polymers in the Rubbery State - DTU Orbit (09/11/2017)

Developing a Macroscopic Mechanistic Model for Low Molecular Weight Diffusion through Polymers in the Rubbery State

Raman microspectroscopy was used to determine the Fickian diffusivity of two families of low molecular weight molecules through amorphous polystyrene in the rubbery state. Different effects of the temperature on diffusivity for each of the families suggested that molecular mobility is controlled by both the volume and flexibility of the diffusing substance when the movement of polymer chains can generate stress induced deformation of molecules. The diffusing molecules were represented as Newtonian spring–bead systems, which allowed us to quantify their flexibility, in function of the vibration frequency of their bonds by reconstructing their theoretical spectra. Results showed that the use of molecular descriptors that take into account flexibility rather than the most stable conformation of the diffusing molecules may improve the description of the diffusion behavior caused by variations in shape and size of the free volumes of the polymeric matrix in the rubbery state.

General information

State: Published
Organisations: National Food Institute, Research Group for Food Production Engineering, Université Montpellier
Authors: Martinez-Lopez, B. (Intern), Huguet, P. (Ekstern), Gontard, N. (Ekstern), Peyron, S. (Ekstern)
Pages: 5078-5089
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information

Journal: Industrial and Engineering Chemistry Research
Volume: 55
Issue number: 17
ISSN (Print): 0888-5885
Ratings:
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.949 SNIP 1.146 CiteScore 2.87
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 0.982 SNIP 1.243 CiteScore 2.6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.066 SNIP 1.338 CiteScore 2.56
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.086 SNIP 1.24 CiteScore 2.58
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.047 SNIP 1.165
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.002 SNIP 1.164
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.142 SNIP 1.267

Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.105 SNIP 1.239
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.035 SNIP 1.204
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.993 SNIP 1.241
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.046 SNIP 1.452
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.101 SNIP 1.266
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.191 SNIP 1.183
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.256 SNIP 1.346
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 1.372 SNIP 1.41
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 1.342 SNIP 1.398
Original language: English
DOIs:
10.1021/acs.iecr.6b00233
Source: FindIt
Source-ID: 2303870813
Publication: Research - peer-review › Journal article – Annual report year: 2016