

## Special Topic on Dynamics of Polymer Materials in Thin Films and Related Geometries

With Guest Editors **Mark Ediger** and **Kenneth Schweizer**

The last twenty years have seen a substantial effort to understand relaxation, mechanics, diffusion, and the glass transition in thin polymer films and related geometries. This special topical brings together an exciting collection of papers utilizing experiment, simulation, and theory, by established and emerging experts in the field. We anticipate that it can play an important role in introducing new researchers to the field and also defining important directions for future work. We are grateful to the authors who contributed manuscripts to this special issue, and see this collection as an important resource for those both inside and outside of the field. The Guest Editors provide some background and perspective in the Preface to the special topic.

### PREFACE

#### Special Topic on Dynamics of Polymer Materials in Thin Films and Related Geometries

M. D. Ediger and Kenneth S. Schweizer  
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### FOCUS

#### Structure and dynamics of the interfacial layer in polymer nanocomposites with attractive interactions

Shiwang Cheng, Bobby Carroll, Vera Bocharova, Jan-Michael Carrillo, Bobby G. Sumpter  
*J. Chem. Phys.* **146**, 203201 (2017)  
DOI: [10.1063/1.4978504](https://doi.org/10.1063/1.4978504)

#### Influence of chemistry, interfacial width, and non-isothermal conditions on spatially heterogeneous activated relaxation and elasticity in glass-forming free standing films

Stephen Mirigian and Kenneth S. Schweizer  
*J. Chem. Phys.* **146**, 203301 (2017)  
DOI: [10.1063/1.4974766](https://doi.org/10.1063/1.4974766)

#### Glassy dynamics of polymethylphenylsiloxane in one- and two-dimensional nanometric confinement—A comparison

Wycliffe K. Kipnusu, Mohamed Elsayed, Reinhard Krause-Rehberg, and Friedrich Kremer  
*J. Chem. Phys.* **146**, 203302 (2017)  
DOI: [10.1063/1.4974767](https://doi.org/10.1063/1.4974767)

#### Reduced-mobility layers with high internal mobility in poly(ethylene oxide)–silica nanocomposites

Yury Golitsyn, Gerald J. Schneider, and Kay Saalwächter  
*J. Chem. Phys.* **146**, 203303 (2017)  
DOI: [10.1063/1.4974768](https://doi.org/10.1063/1.4974768)

#### Unexpected impact of irreversible adsorption on thermal expansion: Adsorbed layers are not that dead

Marie-Luise Braatz, Leslie Infantas Meléndez, Michele Sferrazza, and Simone Napolitano  
*J. Chem. Phys.* **146**, 203304 (2017)  
DOI: [10.1063/1.4974834](https://doi.org/10.1063/1.4974834)

#### Interfacial interaction and glassy dynamics in stacked thin films of poly(methyl methacrylate)

Tatsuhiko Hayashi, Kenta Segawa, Koichiro Sadakane, Koji Fukao, and Norifumi L. Yamada  
*J. Chem. Phys.* **146**, 203305 (2017)  
DOI: [10.1063/1.4974835](https://doi.org/10.1063/1.4974835)

#### Polymer dynamics under cylindrical confinement featuring a locally repulsive surface: A quasielastic neutron scattering study

M. Krutyeva, S. Pasini, M. Monkenbusch, J. Allgaier, J. Maiz  
*J. Chem. Phys.* **146**, 203306 (2017)  
DOI: [10.1063/1.4974836](https://doi.org/10.1063/1.4974836)

#### Local glass transition temperature $T_g(z)$ of polystyrene next to different polymers: Hard vs. soft confinement

Roman R. Baglay and Connie B. Roth  
*J. Chem. Phys.* **146**, 203307 (2017)  
DOI: [10.1063/1.4975168](https://doi.org/10.1063/1.4975168)

#### Relaxation processes and glass transition of confined polymer melts: A molecular dynamics simulation of 1,4-polybutadiene between graphite walls

M. Solar, K. Binder, and W. Paul  
*J. Chem. Phys.* **146**, 203308 (2017)  
DOI: [10.1063/1.4975390](https://doi.org/10.1063/1.4975390)

#### Description of poly(ethylene-propylene) confined in nanopores by a modified Rouse model

Matthias Muthmann, Margarita Krutyeva, Lutz Willner, Jürgen Allgaier, Dieter Richter  
*J. Chem. Phys.* **146**, 203309 (2017)  
DOI: [10.1063/1.4975977](https://doi.org/10.1063/1.4975977)

#### Dynamical heterogeneity in a vapor-deposited polymer glass

Wengang Zhang, Jack F. Douglas, and Francis W. Starr  
*J. Chem. Phys.* **146**, 203310 (2017)  
DOI: [10.1063/1.4976542](https://doi.org/10.1063/1.4976542)

#### Side-group size effects on interfaces and glass formation in supported polymer thin films

Wenjie Xia, Jake Song, David D. Hsu, and Sinan Ketan  
*J. Chem. Phys.* **146**, 203311 (2017)  
DOI: [10.1063/1.4976702](https://doi.org/10.1063/1.4976702)



**Complex nonequilibrium dynamics of stacked polystyrene films deep in the glassy state**

Virginie M. Boucher, Daniele Cangialosi, Angel Alegria, and Juan Colmenero  
*J. Chem. Phys.* **146**, 203312 (2017)  
DOI: 10.1063/1.4977207

**Depth-resolved local conformation and thermal relaxation of polystyrene near substrate interface**

Hung Kim Nguyen, Manabu Inutsuka, Daisuke Kawaguchi, and Keiji Tanaka  
*J. Chem. Phys.* **146**, 203313 (2017)  
DOI: 10.1063/1.4976523

**Interfacial and topological effects on the glass transition in free-standing polystyrene films**

Alexey V. Lyulin, Nikolay K. Balabaev, Arlette R. C. Baljon, Gerardo Mendoza, Curtis W. Frank  
*J. Chem. Phys.* **146**, 203314 (2017)  
DOI: 10.1063/1.4977042

**Dynamics of poly(vinyl methyl ketone) thin films studied by local dielectric spectroscopy**

R. Casalini, M. Labardi, and C. M. Roland  
*J. Chem. Phys.* **146**, 203315 (2017)  
DOI: 10.1063/1.4977785

**The relationship between dynamic and pseudo-thermodynamic measures of the glass transition temperature in nanostructured materials**

Jayachandra Hari Mangalara, Mark E. Mackura, Michael D. Marvin, and David S. Simmons  
*J. Chem. Phys.* **146**, 203316 (2017)  
DOI: 10.1063/1.4977520

**Limited surface mobility inhibits stable glass formation for 2-ethyl-1-hexanol**

M. Tylini, M. S. Beasley, Y. Z. Chua, C. Schick, and M. D. Ediger  
*J. Chem. Phys.* **146**, 203317 (2017)  
DOI: 10.1063/1.4977787

**Network confinement and heterogeneity slows nanoparticle diffusion in polymer gels**

Emmabeth Parrish, Matthew A. Caporizzo, and Russell J. Composto  
*J. Chem. Phys.* **146**, 203318 (2017)  
DOI: 10.1063/1.4978054

**How thermal stress alters the confinement of polymers vitrified in nanopores**

Chao Teng, Linling Li, Yong Wang, Rong Wang, Wei Chen  
*J. Chem. Phys.* **146**, 203319 (2017)  
DOI: 10.1063/1.4978230

**Complex dynamics of capillary imbibition of poly(ethylene oxide) melts in nanoporous alumina**

Yang Yao, Stelios Alexandris, Franziska Henrich, Günter Auernhammer, Martin Steinhart  
*J. Chem. Phys.* **146**, 203320 (2017)  
DOI: 10.1063/1.4978298

**Unexpected behavior of ultra-thin films of blends of polystyrene/poly(vinyl methyl ether) studied by specific heat spectroscopy**

Sherif Madkour, Paulina Szymoniak, Christoph Schick, and Andreas Schönhals  
*J. Chem. Phys.* **146**, 203321 (2017)  
DOI: 10.1063/1.4978505

**The glass transition temperature of thin films: A molecular dynamics study for a bead-spring model**

Craig S. Stevenson, John G. Curro, and John D. McCoy  
*J. Chem. Phys.* **146**, 203322 (2017)  
DOI: 10.1063/1.4977521

**Molecular weight dependence of the intrinsic size effect on T<sub>g</sub> in AAO template-supported polymer nanorods: A DSC study**

Shadid Askar, Tong Wei, Anthony W. Tan, and John M. Torkelson  
*J. Chem. Phys.* **146**, 203323 (2017)  
DOI: 10.1063/1.4978574

**Surface transport mechanisms in molecular glasses probed by the exposure of nano-particles**

Shigang Ruan, Daniele Musumeci, Wei Zhang, Ankit Gujral, M. D. Ediger  
*J. Chem. Phys.* **146**, 203324 (2017)  
DOI: 10.1063/1.4978667

**Direction-dependent elastic properties and phononic behavior of PMMA/BaTiO<sub>3</sub> nanocomposite thin films**

E. Alonso-Redondo, A. Gueddida, H. Huesmann, O. El Abouti, W. Tremel  
*J. Chem. Phys.* **146**, 203325 (2017)  
DOI: 10.1063/1.4978675

**Influence of bidisperse self-assembled monolayer structure on the slip boundary condition of thin polymer films**

Joshua D. McGraw, Mischa Klos, Antoine Bridet, Hendrik Hähl, Michael Paulus  
*J. Chem. Phys.* **146**, 203326 (2017)  
DOI: 10.1063/1.4978676

**Molecular dynamics simulation of the capillary leveling of viscoelastic polymer films**

I. Tanis, H. Meyer, T. Salez, E. Raphaël, A. C. Maggs  
*J. Chem. Phys.* **146**, 203327 (2017)  
DOI: 10.1063/1.4978938

**Using deposition rate to increase the thermal and kinetic stability of vapor-deposited hole transport layer glasses via a simple sublimation apparatus**

Kenneth L. Kearns, Paige Krzyskowski, and Zachary Devereaux  
*J. Chem. Phys.* **146**, 203328 (2017)  
DOI: 10.1063/1.4979814

**The glass transition and enthalpy recovery of a single polystyrene ultrathin film using Flash DSC**

Yung P. Koh and Sindee L. Simon  
*J. Chem. Phys.* **146**, 203329 (2017)  
DOI: 10.1063/1.4979126

**Exploring the broadening and the existence of two glass transitions due to competing interfacial effects in thin, supported polymer films**

Ethan C. Glor, Gabriel V. Angrand, and Zahra Fakhraei  
*J. Chem. Phys.* **146**, 203330 (2017)  
DOI: 10.1063/1.4979944

**Polymer and spherical nanoparticle diffusion in nanocomposites**

Argyrios Karatrantos, Russell J. Composto, Karen I. Winey, and Nigel Clarke  
*J. Chem. Phys.* **146**, 203331 (2017)  
DOI: 10.1063/1.4981258

**Grafted polymer chains suppress nanoparticle diffusion in athermal polymer melts**

Chia-Chun Lin, Philip J. Griffin, Huikuan Chao, Michael J. A. Hore, Kohji Ohno  
*J. Chem. Phys.* **146**, 203332 (2017)  
DOI: 10.1063/1.4982216

**Dynamics of ultra-thin polystyrene with and without a (artificial) dead layer studied by resonance enhanced dynamic light scattering**

S. D. B. Vianna, F. Y. Lin, M. A. Plum, H. Duran, and W. Steffen  
*J. Chem. Phys.* **146**, 203333 (2017)  
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