

Yingrui Shang

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Experience

Computational Instrument Scientist, 1/2021-present
Spallation Neutron Source, Oak Ridge National Laboratory

- Data reduction of small angle neutron scattering for analysis of materials science
- Software package development and maintenance for scientific and industry researchers
- Numerical simulation of polymer materials with verification of
- Publication in scientific research and software technical report

Associate Professor, 1/2012-5/2020
Tianjin University

- Study of structural-property relations with *in-situ* X-ray synchrotron diffraction
- Study in the quantitative correlation of micro-scale structural factors (molecular level) to the mechanical properties with modeling and experiments (SEM/AFM/synchrotron)
- Simulation benchmark and verification with *in-situ* X-ray diffraction.
- Group leader and PI of a research group with 12 students and postdocs

Research Scientist, 9/2009-12/2011
Columbia University, New York, NY

- Multifactor refinement/fitting on massive data of material properties from high energy X-ray and neutron spallation pattern
- Determination of material properties such as lattice parameters, doping, and/or degree of crystallization by Rietveld refinement/fitting
- Leading Software Developer, in Python/C++ for Oak Ridge/Argonne National Laboratory instrument scientists and users, NSF funded project.

Research Assistant, 9/2005-2/2009
University of Massachusetts at Lowell, MA

- Study the phase separation of inhomogeneous ternary polymer blends with finite difference method.
- Optimization of experimental and material variables with models benchmarked by existing results.
- Solving the nonlinear parabolic PDE Cahn-Hilliard Equation with spectral method and developed software for simulation of morphology evolution of polymer blends in 3D in MATLAB

Research & Development Engineer Intern, 5/2007-8/2007, 5/2006-8/2006
Autodesk Inc, Ithaca, NY

- Research and development in algorithms of polymer fluid CAD software (Moldflow, a subsidiary of Autodesk)
- Implement algorithms in FORTRAN/C/C++ to calculate the properties of polymer fluid with short fiber filament. Results verification with experiment data.
- Design and developed the customizable API module in C/C++

Teaching Assistant, 9/2004-9/2005
University of Wyoming, Laramie, WY

- Assisting in assignment grading and class arrangement in Fundamentals of Chemical Engineering

Education

Ph. D in Numerical Modeling of Polymer Physics, obtained in February 2009
University of Massachusetts, 9/2005-5/2009, Lowell, MA

- Dissertation: Numerical simulation of phase separation of ternary polymer blends with surface functionalization with MATLAB. Advisor: Professor David O. Kazmer
- GRE: 2340/2400

- MBA courses: Financial Accounting, Business Finance, and Marketing Fundamentals

B. Sc. in Polymer Science and Material, obtained in June 2004

Beijing University of Chemical Technology, 9/2000-6/2004, Beijing, China

Publications

*Journal papers (corresponding authors are marked with *)*

Cheng Li, **Yingrui Shang***, Huan Xu, Jinqing Li, Shichun Jiang**, " Structure/property relationship of semicrystalline polymers during tensile deformation: a molecular dynamics approach", *Colloid and Polymer Science*, 1-15, 2022

William T. Heller*, John Hetrick*, Jean Bilheux, Jose M. Borreguero, Calvo, Wei-Ren Chen. Lisa De Beer-Schmitt, Changwoo Do, Mathieu Doucet, Michael R. Fitzsimmons, William F. Godoy, Garrett E. Granroth, Steven Hahn, Lilin He, Fahima Islam, Jiao Lin, Kenneth C. Littrell. Marshall McDonnell, Jesse McGaha, Peter F. Peterson, Sai Venkatesh Pingali, Shuo Qian Andrei T. Savici, **Yingrui Shang**, Christopher B. Stanley, Volker S. Urban, Ross E. Whitfield, Chen Zhang, Wenduo Zhou, Jay Jay Billingsa, Matthew J. Cuneo, Ricardo M. Ferraz Leal, Tianhao Wang, Bin Wu, BinWua, "drtans: The data reduction toolkit for small-angle neutron scattering at Oak Ridge National Laboratory", *SoftwareX*, 2022, 19

Huan Xu, **Yingrui Shang***, Xiaoxing Zhang, Jinqing Li, Shichun Jiang**, "Molecular dynamics study in microscopic fundamentals of memory effects of crystalline polymers", to be submitted, 2020

Yingrui Shang, Puqing Ning, Yao Zhang, Feifei Xue, Ziwei Cai, Jinqing Li, Guiqiu Ma, Jian Song, Zhonghua Wu and Shichun Jiang, "Study on structure and property relations of α -iPP during uniaxial deformation via in-situ synchrotron SAXS/WAXS and POM investigations", *Polymer Engineering and Science*, 2018, 58(2)

Bin Wang, **Ying-Rui Shang**, Zhe Ma, Li Pan, and Yue-Sheng Li, "Non-porous ultra low dielectric constant materials based on novel silicon-containing cycloolefin copolymers with tunable performance", *Polymer*, 2017, 116(5)

W Zhang, J Li, **Y Shang**, H Li, S Jiang, L An, "Temperature dependence of tensile behavior in poly (butylene terephthalate) with different crystallinity", *Material & Design*, 2017, 29(5)

Wenyang Zhang, Jinqing Li, **Yingrui Shang**, Hongfei Li, Shichun Jiang, and Lijia An, "Deformation-induced structure evolution of poly(butylene terephthalate)/poly(carbonate) blends during uniaxial stretching", *CrystEngComm*, 2017, 45

Huilong Guo, Chengbo Zhou, Wenyang Zhang, Jiayi Wang, Jinqing Li, **Yingrui Shang**, Yanfeng Meng, Jesper de Claville Christiansen, Donghong Yu, Zhonghua Wu, and Shichun Jiang , "Deformation-induced crystalline structure evolutions of isotactic poly-1-butene", *Colloid and Polymer Science*, 2016, 294

Wenyang Zhang, Chengbo Zhou, Yao Zhang, Feifei Xue, Baojing Luo, Hongfei Li, Xiangkui Ren, Jinqing Li, **Yingrui Shang**, Zhonghua Wu, and Shichun Jiang, "Direct investigations of temperature related structure transitions in strained poly(butylene succinate) with SAXS and WAXS", *Colloid and Polymer Science*, 2016, 294

Jinqing Li, Zhihao Li, Hongyuan Chen, Lili Yang, Huiqin Zheng, **Yingrui Shang**, Donghong Yu, Jesper de Claville Christiansen, and Shichun Jiang, "A qualitative analysis of particle-induced viscosity reduction in polymeric composites", *Journal of Material Science*, 2016, 51

Yingrui Shang, Xiaoxing Zhang, Huan Xu, Jinqing Li, Shichun Jiang*, "Microscopic study of structure/property interrelation of amorphous polymers during uniaxial deformation: A molecular dynamics approach", *Polymer*, 2015,77(23)

Benping Wang, Xianjing Gong, Jinqing Li, **Yingrui Shang**, Dean Shi, Jesper de Claville Christiansen, Donghong Yu, and Shichun Jiang, "Double equilibrium melting temperatures and zero growth temperature of PVDF in PVDF/graphene composites", *Journal of Polymer Research*, 2015, 22(244)

Huilong Guo, Jiayi Wang, Chengbo Zhou, Wenyang Zhang, Zixuan Wang, Bihui Xua, Jinqing Li, **Yingrui Shang**, Jesper de Claville Christiansenc, Donghong Yu, Zhonghua Wu and Shichun Jiang "Direct investigations of deformation and yield induced structure transitions in polyamide 6 below glass transition temperature with WAXS and SAXS", 2015, 70(23)

Jinqing Li, Peitao Xiao, Hongfei Li, Yao Zhang, Feifei Xue, Baojing Luo, Shaoyong Huang, **Yingrui Shang**, Huiying Wen, Jesper de Claville Christiansen, Donghong Yu and Shichun Jiang, "Crystalline structures and crystallization behaviors of poly(l-lactide) in poly(l-lactide)/graphene nanosheet composites", *Polymer Chemistry*, 2015, 21

Jinqing Li, Peipei Guan, Yao Zhang, Feifei Xue, Chengbo Zhou, Jing Zhao, **Yingrui Shang**, Meiling Xue, Donghong Yu and Shichun Jiang, "Shear effects on crystallization behaviors and structure transitions of isotactic poly-1-butene", *Journal of Polymer Research*, 2014, 21(555)

Yingrui Shang, Jing Zhao, Jingqing Li, Zhonghua Wu, Shichun Jiang*, "Investigations in annealing effects on structure and properties of β -isotactic polypropylene with X-ray synchrotron experiments", Colloid and Polymer Science, 2014,292(12)

Lin Liu and **Yingrui Shang**, "Numerical Simulation on Efficiency of Bulk Heterogeneous Junction Solar Cell", Science & Technology Magazine of China Online (open access) , 2014

Yao Zhang, Zhijie Zhang, Hongfei Li, Donghong Yu, **Yingrui Shang**, Lijia An and Shichun Jiang "Influence of Crystallization on Molecular Dynamics of the Amorphous Phase in Poly(ϵ -caprolactone) and Poly(ϵ -caprolactone)/LiClO₄ Complexes Investigated by Dielectric Relaxation Spectroscopy", Journal of Polymer Research, 2013, 20(312)

Shaoyong Huang, Hongfei Li, **Yingrui Shang**, Donghong Yu, Gao Li, Shichun Jiang, Xuesi Chen and Lijia An, "Chloroform micro-evaporation induced ordered structures of poly(L-lactide) thin films", RSC Advances, 2013, 3(33)

Ziwei Cai, Yao Zhang, Jingqing Li, **Yingrui Shang**, Hong Huo, Jiachun Feng, Sergio S. Funari, and Shichun Jiang, "Temperature-dependent selective crystallization behavior of isotactic polypropylene with a β -nucleating agent", Journal of Applied Polymer Science, 2013, 128(1)

Peitao Xiao, Hongfei Li, Shaoyong Huang, Huiying Wen, Donghong Yu, **Yingrui Shang**, Jingqing Li, Zhonghua Wu, Lijia An and Shichun Jiang, "Shear Effects on Crystalline Structures of Poly(L-lactide)", CrystEngComm, 2013, 39

Huilong Guo, Yao Zhang, Feifei Xue, Ziwei Cai, **Yingrui Shang**, Jingqing Li, Yu Chen, Zhonghua Wu and Shichun Jiang, "In-situ synchrotron SAXS and WAXS investigations on deformation and α - β transformation of uniaxial stretched poly(vinylidene fluoride)", CrystEngComm, 2013, 8

Peng Tian, Wenduo Zhou, Jiwu Liu, **Yingrui Shang**, Chris Farrow, Pavol Juhas, Simon Billinge*, "SrRietveld: a program for automating Rietveld refinements for high-throughput powder diffraction studies", Journal of Applied Crystallography, 2013, 46.

Hong Huo, Xuemin Yao, Yao Zhang, Jingqing Li, **Yingrui Shang** and Shichun Jiang, "In situ studies on the temperature-related deformation behavior of isotactic polypropylene spherulites with uniaxial stretching: The effect of crystallization conditions", Polymer Engineering and Science, 2013, 53(1)

Liang Fang, Ming Wei, **Yingrui Shang**, David Kazmer, Carol Barry and Joey Mead*, "Precise Pattern Replication of Polymer Blends into Nonuniform Geometries via Reducing Interfacial Tension between Two Polymers", Langmuir, 2012, 28(27)

Hu Ping Mao, Hongfei Li, **Yingrui Shang**, Jingqing Li, Conghua Lu, Lijia An and Shichun Jiang, "Solvent vapor induced structural evolution of micelle clusters and square slices that form in PS-b-PEO solutions", Journal of Polymer Research, 2012, 19(11)

Yao Zhang, Hong Huo, Jingqing Li, **Yingrui Shang**, Yu Chen, Sergio S. Funari and Shichun Jiang, "Crystallization behavior of poly(ϵ -caprolactone) and poly(ϵ -caprolactone)/LiClO₄ complexes from the melt", CrystEngComm, 2012(23)

Ziwei Cai, Yao Zhang, Jingqing Li, Feifei Xue, **Yingrui Shang**, Xuehao He, Jiachun Feng, Zhonghua Wu and Shichun Jiang, "Real time synchrotron SAXS and WAXS investigations on temperature related deformation and transitions of β -iPP with uniaxial stretching", Polymer, 2012, 53(7)

Jingqing Li, Yao Zhang, Yundan Jiacao, **Yingrui Shang**, Hong Huo and Shichun Jiang, "Miscibility and rheologically determined phase diagram of poly(ethylene oxide)/poly(ϵ -caprolactone) blends", Polymer Bulletin, 2012, 68

Yingrui Shang and David Kazmer, "A MATLAB programme for quantitative simulation of self-assembly of polymer blend films with nanoscaled features", International Journal of Computer Aided Engineering and Technology, 2012, 4(2)

Yingrui Shang*, David Kazmer*, Ming Wei, Carol Barry, and Joey Mead, "Verification of Numerical Simulation of the Self-assembly of a Polymer-polymer-solvent Ternary Blends on a Heterogeneously Functionalized Substrate", Polymer, 2011, 52(6)

Yingrui Shang and David Kazmer, " A MATLAB Program for Quantitative Simulation of Self-assembly of Polymer Blend Films with Nano-scaled Features", Arxiv/Material Science, 2010

Liang Fang, Ming Wei, **Yingrui Shang**, Lady Jimenez, David Kazmer, Carol Barry and Joey Mead, "Surface morphology alignment of block copolymers induced by injection molding", Polymer, 50(24), 2009

Yingrui Shang*, David Kazmer*, Ming Wei, Carol Barry, and Joey Mead, "Numerical Simulation of Phase Separation of a Polymer-polymer-solvent Ternary Blend on a Heterogeneously Functionalized Substrate", Polymer Engineering and Science, 2010, 50(12)

Yingrui Shang, David Kazmer, Ming Wei, Joey Mead, and Carol Barry, "Numerical Simulation of Phase Separation of Immiscible Polymer Blends on a Heterogeneously Functionalized Substrate", *The Journal of Chemical Physics*, 128(22), 2008

Books and Chapters

Yingrui Shang* and David Kazmer* (2014), Chapter 3: Modeling and Simulation, in "Characterization of Polymer Blends: Miscibility, Morphology and Interfaces" p457-522, Weinheim, Germany. Wiley-VCH Verlag GmbH & Co

Yingrui Shang, "Numerical Simulation of the Phase Separation of a Polymer-Polymer-Solvent Ternary System on a Heterogeneously Functionalized Substrate", dissertation, University of Massachusetts at Lowell, 2009

Conference papers and presentations

Yingrui Shang, Cheng Li and Shichun Jiang, "Molecular dynamics simulation of structure and property relation of crystallized polymer during uniaxial deformation", Polymer Crystallization Youth Forum, September 2016, Zhengzhou, presentation

Yingrui Shang, "Numerical simulation and data processing on polymer materials", Academic Salon, January 2015, Tianjin, presentation

Yingrui Shang, Xiaoxing Zhang and Shichun Jiang, "Molecular dynamics simulation of amorphous polymer during uniaxial deformation", Polymer Material and Engineering Conference, October 2014, Chengdu, presentation

Yingrui Shang, Xiaoxing Zhang and Shichun Jiang, "Analysis on Effects of Structural Evolution during Uniaxial Deformation of Amorphous Polymers", Chinese Chemical Society 2014: Polymer System Theory, Simulation and Modeling Conference, June 2014, Changchun, presentation

Yingrui Shang, Xiaoxing Zhang, Shuaichao Zhang and Shichun Jiang, "Molecular dynamics simulation of polymer during deformation", 2013 National Polymer Conference of China, Shanghai, 2013 October, presentation

Yingrui Shang, "Numerical simulation on phase separation of ternary polymer blends", December, 2013, National Key Laboratory of Composites Annual Conference, invited talk

Yingrui Shang and David Kazmer, "Validation of Numerical Simulation of Polymer Self-assembly on Patterned Substrate", National Science Foundation site visit on Center of High-rate Nanomanufacturing, Lowell, MA, presentation report, June, 2008,

Yingrui Shang, Ming Wei, Carol Barry, Joey Mead, and David Kazmer, "Numerical Simulation of Composition Induced Phase Separation in a Polymer-polymer-solvent Ternary System on a Patterned Substrate with Nano Features", 2008 ASME International Mechanical Engineering Congress and Exposition, Speaker, November, 2008.

Yingrui Shang, Ming Wei, David Kazmer, Joy Mead, and Carol Barry, "Numerical Simulation of Polymer Phase Separation on a Patterned Substrate with Nano Features", Nano Science and Technology Institute, Nanotech 2008, Speaker, June 2008.

Liang Fang, Ming Wei, **Yingrui Shang**, Jun S.Lee, Carol Barry, David Kazmer, and Joey Mead, "The Effect of Mold Temperature on the Surface Phase Morphology of Injection Molded Block Copolymer", the 235th American Chemical Society National Meeting, April 8-11, 2008

Yingrui Shang, Ming Wei, David Kazmer, Joey Mead, and Carol Barry, "Experimental validation of numerical simulation for phase decomposition of a binary polymer thin film on a patterned substrate", ANTEC Annual Technical Conference, Speaker, May 2007.

Yingrui Shang and David Kazmer, "Numerical Simulation of Polymer Phase Separation on Patterned Substrate", National Science Foundation site visit on Center of High-rate Nanomanufacturing, Boston, MA, poster session, June, 2007,

Yingrui Shang and David Kazmer, "Modeling of Spinodal Decomposition of Polymer Blends", National Science Foundation site visit on Center of High-rate Nanomanufacturing, Durham, NH, poster session, June, 2006,

Yingrui Shang and David O. Kazmer, "Simulation of Polymer Morphology in Nano-feature Replication", Sukant Tripathy Annual Memorial Symposium 2005, Sept. 22, 2005, poster session.

Yingrui Shang and David O. Kazmer, "Numerical Simulation of Phase Separation of Polymer Blends near Patterned Substrate", US Japan Young Researchers Conference, Feb. 27, 2006, poster session.

Activities and Duties

Principal Investigator in multiple scientific research funds from NSFC

Reviewer, *Journal of Applied Polymer Science*

Co-chair, 2009 AIChE Annual Meeting

Reviewer, Langmuir, American Chemical Society
Member, IEEE
Member, Society of Plastics Engineers
Member, American Society of Mechanical Engineers

Awards

Outstanding mentor, Tianjin University College of Material Science and Engineering, 2015
Top 30 in E-commerce startup, Heimai Venture Competition (national), 11/2012
Outstanding Presenter, Society of Advancement of Material and Process Engineering, 2007
Outstanding Student, MSE at Beijing University of Chemical Technology, 2000-2004
2nd Grade People's Scholarship, Beijing University of Chemical Technology, 2000-2004

Funding

Principle Investigator, National Science Foundation of China
2013/1-2015/12, ¥ 250,000, 2120406: Molecular dynamics simulation and experimental verification of structure evolution of semicrystalline polymer materials during deformation
Principle Investigator, New Scholar Fund, Department of Education of China
2013/1-2015/12, ¥ 40,000, 20120032120018, Numerical simulation study of structure property relation of bulk hetero-junction organic solar cells
Principle Investigator, New Century Excellence Financial Support, Tianjin University
2013/1-2014/12, ¥ 50,000, 1308, Validation of molecular dynamics simulation of deformation of isotactic-polypropylene
Unfunded
Principle Investigator, National Science Foundation of China
2016/1-2019/12, ¥ 800,000, 2167040: A molecular dynamics study on the melt memory effect in polymer crystallization

Research Advising

Graduate Student

Cheng Li, "Molecular dynamics simulation in crystalline polymer deformation", 2018
Huan Xu, "Molecular dynamics simulation in crystallization of polymer", 2016 - Procter & Gamble
Xiaoxing Zhang, "Molecular dynamics in polymer deformation", 2015 - Beijing Hyundai
Jing Zhao, "X-ray diffraction study on beta-iPP deformation", 2013

Undergraduate Thesis

Guanye Huang, "Influence of chain conformation and meso-structure on property of hydrogel", 2018
Yunyi Ma, "Molecular dynamics simulation of melt-memory effect of polymer materials", 2017
Jiaxi Zhao, " Polyacrylamide hydrogel structure and property relations modeling", 2017
Rui Guan, "Molecular dynamics study of graphene/polymer composites properties", 2016
Zhijiang Che, "Molecular dynamics simulation of deformation of crystallized polymer", 2016
Ning Cao, "Molecular dynamics simulation of polymer crystallization", 2015
Jiahui Cui, "Molecular dynamics study of deformation of polypropylene", 2015
Meng Su, "Gradients of durable PVC cable cover for wind power generator", 2014
Lin Liu, "Numerical simulation of structure-efficiency relation of BHJ organic solar cell", 2014
Deji Ciren, "X-ray diffraction investigation on structure property relation of iPP", 2014
Liao Chen, "Molecular dynamics simulation of relaxation of polymer", 2014
Qingli Pei, "Modeling in structure-property relation of bulk hetero-junction organic solar cell", 2013
Xuedan Liu, "Numerical study on polymer materials with negative Poisson ratio", 2013
Shuaichao Zhang, "Molecular dynamic simulation on polymer during deformation", 2013

Funded Student Research Project

Xiaolu Chen, "Molecular dynamics simulation of crystallized polymer during deformation",
2013/6-2014/6, ¥ 6956.52

Teaching

Experiment in Polymer Physics, undergraduate, 2014-2019
Polymer Design and Experiment, undergraduate, 2016-2018

Polymer Physics, undergraduate, 2012-2014
Numerical Method in Material Science, graduate, 2012-2016
Fundamental in Chemical Engineering Experiment, undergraduate, 2004 as teaching assistant

University Involvement

Committee Member, Graduate Student Admission in College of MSE, 2012-2019
Committee Member, Undergraduate Student Thesis Evaluation in College, 2012-2019
Presenter, Undergraduate Student Enrollment, 2016-2019
Committee Member, Undergraduate Innovation Project, 2014-2019
Committee Member, Polymer Physics Experiment Class Reformation, 2014-2019
Faculty Fellow, Academic Summer Camp, 2014-2018
Coordinator, Dept. of Tech. 973 Funding Initiation, 2014
Faculty Mentor, Undergraduate MSE Class 2009-2014, 2013-2018

Activities and Adventures

Comments and reviews, World Journal Newspaper, 2006-2008
President, Graduate Student Association, University of Massachusetts, Lowell, 2006-2007
Columnist, "Another Home", *Hebei Pictures* (weekly), 2005-2007
President, Chinese Student and Scholar Association, UMass Lowell, 2006-2007
College Basketball Team, Point Guard, Beijing Univ. of Chemical Technology, 2000-2003
Best Comedian/Play Writer, "You and Me, in 10 Years", BUCT, 2003
Editor, *Polymer Student* (monthly), BUCT, 2000-2003
High School Basketball Team, Point Guard, Hengshui Middle High, 1997-2000

Personal Information

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