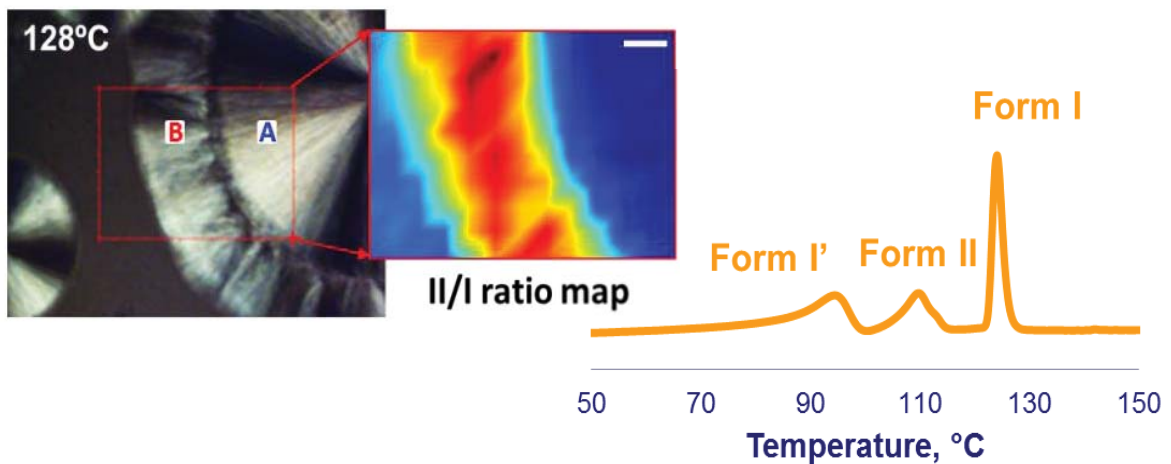


WORKSHOP ON POLYMER CRYSTALLIZATION

4th edition

Genova, 3-5 September 2018

PROCEEDINGS



Venue: Chierici Hall, Biblioteca Berio, Via del Seminario, 16 Genova

Organizers:

Dario Cavallo, Giovanni Carlo Alfonso and Gerrit W.M. Peters

Local organization

Adriana Saccone, Silvia Vicini, Maila Castellano, Orietta Monticelli, Davide Comoretto, Paola Lova, Bao Wang, Seif Fenni

Scientific Committee

Giovanni Carlo Alfonso, Luigi Balzano, Markus Gahleitner, Wenbing Hu, Alejandro Jesus Müller

Sponsorships:

**Polymer
Crystallization**



WORKSHOP TIMETABLE at GLANCE

(as in August 22, 2018)

	Monday, Sept. 3 rd			Tuesday, Sept. 4 th		Wednesday, Sept. 5 th	
8.30-9.00	Registration						
9.00-9.10	Opening		9.00-9.40	I3	Li	9.00-9.40	I5 Thurn-Albrecht
9.10-9.50	I1	Yan	9.40-10.00	O13	Ivanov	9.40-10.00	O25 Gohn
9.50-10.10	O1	Zeng	10.00-10.20	O14	Vanzanella	10.00-10.20	O26 Grosso
10.10-10.30	O2	Lotz	10.20-10.40	O15	Lova	10.20-10.40	O27 Hu
10.30-11.00	COFFEE BREAK		10.40-11.10	COFFEE BREAK		10.40-11.10	COFFEE BREAK
11.00-11.20	O3	Looijmans	11.10-11.30	O16	Perez Camargo	11.10-11.30	O28 Pantani
11.20-11.40	O4	Ma	11.30-11.50	O17	Goderis	11.30-11.50	O29 Rhoades
11.40-12.00	O5	Paolucci	11.50-12.10	O18	Boragno	11.50-12.10	O30 Boyer
12.00-12.20	O6	Krajenta	12.10-12.30	O19	Harings	12.10-12.50	I6 Balzano
			12.30-13.00	O20	Fulchiron	12.50-13.00	Closing remarks
12.20-12.40	O7	Schäfer	13.00-14.30	LUNCH		13.00-14.30	LUNCH
12.40-13.00	O8	Meille	14.30-15.10	I4	Mileva		
13.00-14.30	LUNCH + posters hang up		15.10-15.30	O21	Galeski		
14.30-15.10	I2	De Rosa	15.30-15.50	O22	Di Lorenzo		
15.10-15.30	O9	Müller	15.50-16.10	O23	Boyard		
15.30-15.50	O10	Pan	16.10-16.40	COFFEE BREAK			
15.50-16.10	O11	Tranchida	16.40-17.00	O24	Fernandez-Ballestrer		
16.10-16.40	COFFEE BREAK		17.00-18.30	POSTERS READING + posters removal			
16.40-17.00	O12	Malizia					
17.00-18.30	POSTERS READING						

Modelling crystalline phase transitions in poly(3-alkylthiophenes)

Mosè Casalegno, Antonino Famulari, Guido Raos, Stefano Valdo Meille

Dipartimento di Chimica, Materiali e Ingegneria Chimica "Giulio Natta", Politecnico di Milano

The ways polymers respond reorganizing structurally, or else recrystallize, because of thermal or pressure treatments, or irradiation, or electrical stimulation, etc., are of basic interest. Except in very rare cases, it is however impossible to follow experimentally these transitions, except for slow processes, or more generally, for selected features. On the other hand, complete structural models are accessible only for the initial and final structures. Organic polymers for optoelectronics applications represent an extreme case in the above scenario because they normally organize poorly in the solid state. It is consequently difficult even to devise sensible initial and final models for structural transitions.¹ This depends on key features of their molecular structure, which, is characterized by a π -conjugated main chain, essential for charge transport, and relatively long alkyl side chains, that make these materials processable. In transitions involving such molecules, the new structures evolve by a negotiation involving the different main chain and side chain properties, leading in some instances to microphase-segregated structures.

We will report on poly(3-alkylthiophenes) (P3ATs), because on one hand they are a simple but fully representative family of conjugated polymers. On the other hand, they have been extensively studied for decades.² Atomistic molecular dynamics (MD) simulations of experimentally observed transitions of various P3ATs, from selected ordered states to more disordered structures, which, under appropriate circumstances can be followed continuously. The study has been made possible by the development of a force-field adapted for P3ATs,³ and by the identification of selected reliable starting models.³⁻⁵ The molecular assemblies resulting from the simulation process display substantial reorganization, leading to development of dislocations and of stacking defects of various kind, in part frozen in upon cooling the models. The observed, plausibly entropy driven, transitions will be discussed in the context of polymer phase transition modeling.

1. J. Rivnay, S. C. B. Mannsfeld, C. E. Miller, A. Salleo, M. F. Toney, *Chem. Rev.* 112, 5488 (2012).
2. M. Brinkmann, *J. Polym. Sci., Part B: Polym. Phys.* 49, 1218 (2011).
3. M. Moreno, M. Casalegno, G. Raos, S. V. Meille, R. Po, *J. Phys. Chem. B*, 114, 1591 (2010).
4. P. Arosio, M. Moreno, A. Famulari, G. Raos, M. Catellani, S. V. Meille, *Chem. Mater.* 21, 78 (2009).
5. A. Buono, N. H. Son, G. Raos, et al., *Macromolecules* 43, 6772 (2010).