

MS43-P3 Structural characterization of a [1]benzothieno [3,2-b]benzothiophene (btbt) derivative in bulk and thin films

Gabin Gbabode¹, Aurelien Blangenois¹, Philippe Négrier², Denise Mondieig², Gérard Coquerel¹, Yves Geerts³, Michele Sferrazza⁴

1. Unité de Cristallogénèse, SMS, EA 3233, Normandie Université, Université de Rouen, 1 rue Lucien Tesnière, F-76821 Mont-Saint-Aignan, France

2. Université Bordeaux, LOMA, UMR 5798, 351 Cours de la Libération, F-33400 Talence, France

3. Laboratoire de Chimie des Polymères, Faculté des Sciences, Université Libre de Bruxelles CP206/1, Campus de la Plaine, B-1050 Brussels, Belgium

4. Département de Physique, Faculté des Sciences, Université Libre de Bruxelles CP223, Campus de la Plaine, B-1050 Brussels, Belgium

email: gabin.gbabode@univ-rouen.fr

In the past decades, particular attention has been paid onto organic molecules comprising π -conjugated moieties owing to their potential applications in the promising field of organic electronics [1]. In this framework, knowledge of the crystal packing of target molecules is of prime importance since charge transport properties are highly dependent on the structural arrangement. Furthermore, it has been demonstrated that charge transport is effectively driven by the first molecular layers close to the underlying substrate in the case of Organic Field-Effect Transistors (OFETs) [2]. Then, structural characterization studies aiming at seeking eventual polymorphism in thin films and understanding its occurrence are mandatory for a rational design of devices architecture.

In this presentation, we will show results on the polymorphism of a mono-alkylated (with an octyl chain) [1]benzothieno[3,2-b]benzothiophene molecule (hereafter called C8-BTBT) in bulk samples and thin films. Alkylated BTBT molecules are currently among the most promising candidates to be used as solution-processed air-stable high-performance organic semiconductors [3].

We proved the existence of three distinct polymorphs for C8-BTBT bulk samples, called forms I, II and III, forms I and III being observed at room temperature and form II at high temperature. The crystal structures of forms I and III have been determined from X-ray powder diffraction data and both consist in lamellar arrangement composed of bi-layers of “head-to-head” (or “tail-to-tail”) stacked molecules.

Grazing incidence X-ray diffraction measurements on C8-BTBT thin films showed that the same structural arrangement is revealed in all thin films independently of film thickness and corresponds to form III observed for bulk samples, then discarding the possibility of a substrate-induced phase [4] for this compound. A tentative explanation of this result will be given in our presentation based on the crystal structure determined for form III.

References.

[1] A. Facchetti, *Materials Today* 2007, 10, 28-37.

[2] F. Dinelli, M. Murgia, P. Levy, M. Cavallini, F. Biscarini, D. M. de Leeuw, *Phys. Rev. Lett.* 2004, 92, 116802.

[3] Y. Yuan, G. Giri, A. L. Ayzner, A. P. Zoombelt, S. C. B. Mannsfeld, J. Chen, D. Nordlund, M. F. Toney, J. Huang, Z. Bao, *Nat. Commun* 2014, 5, 3005-3013.

[4] G. Gbabode, N. Dumont, F. Quist, G. Schweicher, A. Moser, P. Viville, R. Lazzaroni, Y. H. Geerts, *Adv. Mater.* 2012, 24, 658-662.

Keywords: polymorphism, thin films, grazing incidence X-ray diffraction, crystal structure determination, organic electronics.