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Theo Rasing

Radboud University, Netherlands

Jumping crystals: Controlled giant thermoelastic deformation of an organic molecular crystal

Thermosalient molecular crystals are characterized by thermally induced single crystal to single crystal phase transitions that are accompanied by sudden anisotropic lattice expansion, giving rise to huge mechanical responses to external stimuli: upon heating or cooling they jump distances many times their own size. This makes these materials invaluable for the design of a new generation of switchable smart materials which are central to, e.g., soft robotics, artificial muscles and microfluidic valves. The abrupt and strong macroscopic shape changes are connected to a structural phase transition inside such crystals. However, the detailed mechanisms of these phase transitions are unknown. In addition, the large changes in crystal shape and size is difficult to accommodate for the often brittle organic crystals and the mechanical effects are usually accompanied by crystal cracking, splitting or even explosion. Here, we report on a layered crystal structure of the fluorenone derivative 4-DBpFO, clearly showing a strong and reproducible shear deformation when it undergoes a structural phase transition upon heating. Moreover, this shear deformation can be observed along two orthogonal crystal directions, which appears to be connected to its crystal structure. The deformation of the single crystal can be controlled by heating/cooling cycles without destroying it. Modelling shows that the shear deformation that accompanies the in-plane anisotropic lattice expansion results from in-plane molecular rotations during the phase transition and follows a nucleation and growth path. We believe that 4-DBpFO could serve as a model structure to guide the development of new types of robust thermosalient organic crystals.

Recent Publications

1. X Li et al. (2018) Strong optical nonlinearities of self-assembled polymorphic microstructures of phenylmethyl functionalized fluorones. Chin. Chem. Lett. 29:297-3000.
2. Y Luo et al. (2017) Controlling the growth of molecular crystal aggregates with distinct linear and nonlinear optical properties. ACS Applied Materials & Interfaces 9:30862-30871.
3. Thibault Chervy, Jialiang Xu, Yulong Duan, Chunliang Wang, Loïc Mager, Maurice Frerejean, Joris A W Münninghoff, Paul Tinnemans, James A Hutchison, Cyriaque Genet, Alan E Rowan, Theo Rasing and Thomas W Ebbesen (2016) High-efficiency second-harmonic generation from hybrid light matter states. Nano Letters 16:7352-7356.
4. J Xu et al. (2016) Advances in soft functional materials research. Adv. Funct. Mat. 26:8807-8809.
5. A Kirilyuk, A Kimel and Th Rasing (2010) Ultrafast optical manipulation of magnetic order. Rev. Mod. Phys. 82:2731-2784.

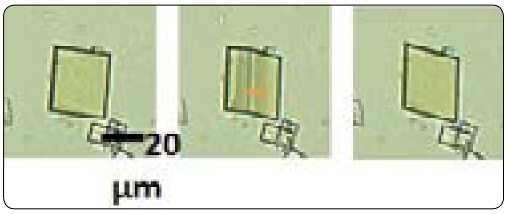

Figure 1: Microscopic images showing the shear deformation of a planar quadrangular single crystal (left) to a diamond shape (right) during the α- to β-phase transformation of 4-DBpFO. The arrow in the middle picture indicates the movement of the phase boundary.

Biography

Theo Rasing is a full Professor of Physics at Radboud University, Nijmegen. He is the Elected Member of the Royal Dutch Academy of Arts and Sciences (KNAW) and the Academia Europaea. He is an Honorary Member of the Ioffe Institute in St. Petersburg; Knight of the Order of the Dutch Lion and recipient of many scientific prices and awards, including an ERC Advanced Grant 2013, the Spinoza Award 2008, and the Prize for Science and Society 2008. His research focuses on the investigation and control of the properties of functional (molecular/photonic) nanomaterials on ultrafast (femtosecond) timescales. He has co-authored over 480 papers with over 12000 citations (h index 54, Web of Science). His publications include 41 articles in *Physical Review Letters* and 15 in *Nature Group Journals*. One of the *Physical Review Letters* of 2007 was mentioned as one of the breakthroughs of the year by the journal Science. He is a Co-Inventor on 3 patent applications.

th.rasing@science.ru.nl