

KN06

Acta Cryst. (2011) A67, C7**Crystalline molecular flasks**

Makoto Fujita *Department of Applied Chemistry, School of Engineering, The University of Tokyo, Tokyo 113-8656 (Japan).* E-mail: mfujita@appchem.t.u-tokyo.ac.jp

Since our first report on a zeolite-mimic coordination network in 1994,[1] we have developed several robust coordination network complexes possessing large pores.[2-8] In some cases, the pore channels facilitate increased mobility and rapid diffusion of included guest molecules. Large organic molecules can easily enter into the pores via guest exchange. In this sense, the pore interior is a pseudo-solution state where chemical reactions may proceed as in a solution, yet can be directly analyzed by crystallography. Here, we show that single-crystal-to-single-crystal chemical reactions with large, common reagents proceed quite smoothly inside the pores of the network.[9] Taking advantage of the network's robust crystallinity, we succeeded in the acylation and ureidation of aromatic amines and imine formation from aromatic aldehydes within a single crystal. The pores of the network complexes thus serve as "crystalline molecular flasks". We also show a hemiaminal, a transient short-lived intermediate in the Schiff-base formation, can be trapped and directly observed by X-ray analysis in the crystalline molecular flasks.[10]

[1] M. Fujita, Y.-J. Kwon, S. Washizu, K. Ogura, *J. Am. Chem. Soc.* **1994**, *116*, 1151. [2] K. Biradha, M. Fujita, *Angew. Chem. Int. Ed.* **2002**, *41*, 3392. [3] O. Ohmori, M. Kawano, M. Fujita *J. Am. Chem. Soc.* **2004**, *126*, 16292. [4] K. Takaoka, M. Kawano, M. Tominaga, M. Fujita *Angew. Chem. Int. Ed.* **2005**, *44*, 2151. [5] O. Ohmori, M. Kawano, M. Fujita, *Angew. Chem. Int. Ed.* **2005**, *44*, 1962. [6] M. Kawano, T. Kawamichi, T. Haneda, T. Kojima, M. Fujita, *J. Am. Chem. Soc.* **2007**, *129*, 15418. [7] T. Haneda, M. Kawano, T. Kojima and M. Fujita *Angew. Chem. Int. Ed.* **2007**, *46*, 6643. [8] T. Haneda, M. Kawano, T. Kawamichi, M. Fujita, *J. Am. Chem. Soc.* **2008**, *130*, 1578. [9] T. Kawamichi, T. Kodama, M. Kawano, M. Fujita, *Angew. Chem. Int. Ed.* **2008**, *47*, 8030. [10] T. Kawamichi, T. Haneda, M. Kawano, M. Fujita, *Nature* **2009**, *461*, 633.

Keywords: inclusion, reaction, coordination

KN07

Acta Cryst. (2011) A67, C7**Microtubule-Kinetochore Interactions**

Eva Nogales^a, Greg Alushin^b, Vincent Ramey^b. ^a *MCB Department, UC Berkeley, HHMI.* ^b *Biophysics Graduate Program, UC Berkeley (USA).* E-mail: enogales@lbl.gov

During division the eukaryotic cell needs to accurately segregate its genetic material between daughter cells. This process involves the interaction of the microtubule mitotic spindle with special regions on chromosomes called kinetochores. Errors, which result in misplaced chromosomes, can lead to cancer or death. We have visualized the interaction of microtubules with two kinetochore components, the yeast Dam1 and the human Ndc80 complexes, using cryo-electron microscopy and image reconstruction.

The Dam1 kinetochore complex is essential for chromosome segregation in budding yeast. It is a ten-protein complex that self-assembles around microtubules, forming ring-like structures that move with depolymerizing microtubule ends, a mechanism with implications for cellular function [1], [2]. We have defined the architecture of the Dam1 complex, at about 30-Å resolution, both in its unbound and microtubule-bound states [3].

The Ndc80 complex is a key site of regulated kinetochore-microtubule attachment, conserved from yeast to humans. We have

obtained a subnanometre-resolution reconstruction of the human Ndc80 complex bound to microtubules, and docked the crystal structures of the component proteins [4]. The Ndc80 complex binds the microtubule with a tubulin monomer repeat, recognizing α - and β -tubulin at both intra- and inter-tubulin dimer interfaces in a manner that is sensitive to tubulin conformation. Ndc80 complexes self-associate along protofilaments forming linear arrays.

Formation of both kinetochore complex oligomers is regulated by Aurora B phosphorylation, so that wrong attachments can be corrected. Our structures and biophysical and biochemical studies [5], [6] lead to mechanistic models of how the kinetochore machinery is capable of harnessing microtubule depolymerization for chromosome movement.

[1] S. Westermann, A. Avila-Sakar, H.W. Wang, H. Niederstrasser, J. Wong, D.G. Drubin, E. Nogales, and G. Barnes, *Mol Cell* **2005**, *17*, 277-90. [2] S. Westermann, H.W. Wang, A. Avila-Sakar, D.G. Drubin, E. Nogales, and G. Barnes, *Nature* **2006**, *440*, 565-9. [3] H.W. Wang, V.H. Ramey, S. Westermann, A.E. Leschziner, J.P. Welburn, Y. Nakajima, D.G. Drubin, G. Barnes, and E. Nogales, *Nat Struct Mol Biol* **2007**, *14*, 721-6. [4] G.M. Alushin, V.H. Ramey, S. Pasqualato, D.A. Ball, N. Grigorieff, A. Musacchio, and E. Nogales, *Nature* **2010**, *467*, 805-810. [5] H.W. Wang, S. Long, C. Ciferri, S. Westermann, D. Drubin, G. Barnes, and E. Nogales, *J Mol Biol* **2008**, *383*, 894-903. [6] V.H. Ramey, H.W. Wang, Y. Nakajima, A. Wong, J. Liu, D. Drubin, G. Barnes, and E. Nogales, *Mol Biol Cell* **2011**, *22*, 457-66.

Keywords: Ndc80, Dam1, cryo-EM

KN08

Acta Cryst. (2011) A67, C7-C8**Use of external fields in the melt growth of semiconductors**

Roberto Fornari, *IKZ – Leibniz Institute for Crystal Growth, Berlin and Physics Dept., Humboldt University, Berlin.* E-mail: fornari@ikz-berlin.de

Stationary and non-stationary magnetic fields have been widely applied for the melt growth of semiconductors in order to control the convection within the crucibles. Indeed when scaling up to industrial equipments, with melt masses above 200 Kg, the relatively large thermal gradients within the crucibles result in strong convective flows which ultimately degrade the quality of the semiconductor crystals. In some case, under very unfavorable conditions, even onset of turbulence was observed. Pronounced striations, incorporation of undesired impurities coming from the crucible/ambient and doping non-uniformity are the typical defects. In standard experimental setups, such as Czochralski or Bridgman furnaces, the magnetic fields provided by one or more electromagnetic coil(s) placed around the growth chamber, in correspondence of the crucible position, may effectively damp the convective motion. However, although capable of reducing the convection of the melt, this type of setup has hardly met the expectations of academic and industrial crystal growers due to the cost of the magnet(s) and the high energy consumption. As a matter of fact the use of magnetic field has so far been treated almost as a laboratory curiosity. Just in the case of very large melt amounts (typically CZ growth of silicon), where the elevated Rayleigh number leads to strong turbulence and negatively impacts the single crystal growth, the magnetic field found practical application.

At IKZ, in the frame of the KristMAG[®] consortium, an alternative approach was developed. In this case the resistive heaters of two CZ pullers and one VFG furnace were substantially modified in order to simultaneously provide heat and magnetic field to the melt [1, 2, 3]. This is possible by adopting a spiral configuration for the graphite heaters and by simultaneously feeding these coils with DC and AC currents. The DC current essentially determines the temperature set point, whereas the AC signal provides a so-called *travelling magnetic*