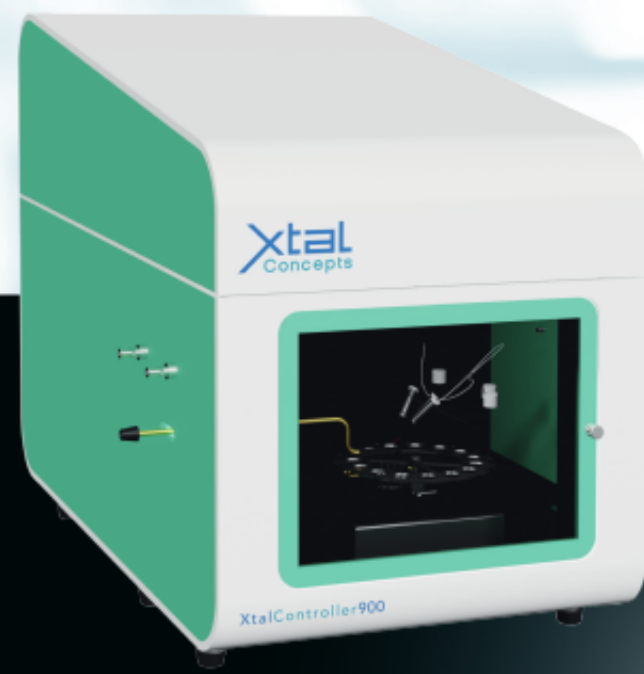
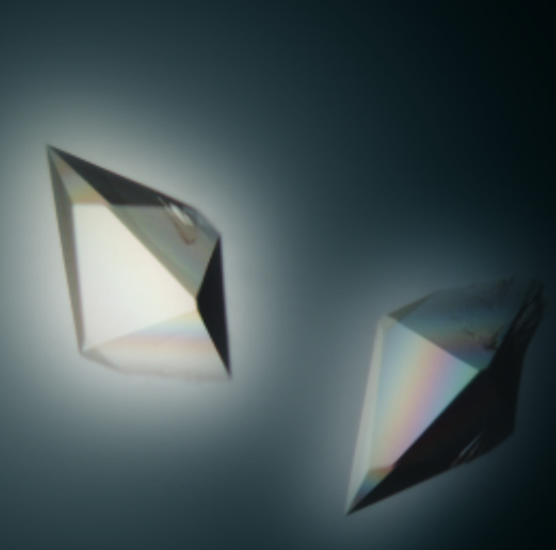




XtalController 900

The Patented Interactive Crystallization System

XtalController 900

is used either as an analytical device to optimize crystallisation conditions or for production of crystals of various dimensions. It allows actively drop composition changes by picoliter titration via piezo controlled drop dispensers. All fundamental drop parameters are known and can be controlled at all times of the experiment.

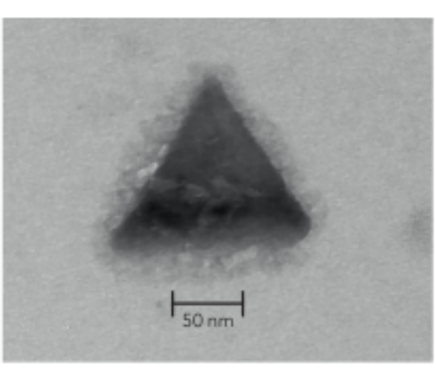
PRESENTED SOLUTION

- Manoevering through the phase diagram
- Tuning of crystal dimensions
- Production of nano crystals by intervention in the nucleation process

UNIQUE FEATURES

- Concentration monitoring via micro balancing
- Controlled evaporation
- Active precipitant concentration control and change via micro dosage systems
- Nucleation and nanocrystal detection via DLS
- Drop imaging

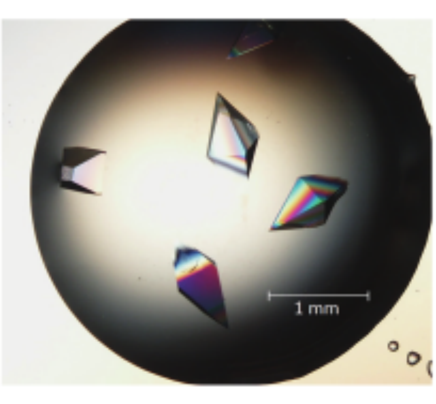
Most Frequent Applications of Interactive Crystallization



NANOCRYSTAL PRODUCTION

The response of a protein to an increasing concentration of precipitant is often quite dramatic although the drop remains fully clear. Among all kinds of protein responses nucleation is characterised by a unique signature.

- DLS monitoring of nucleation or clustering
- Monitoring the transition of liquid dense clusters to nanocrystals
- Fully automated experiment conduction
- Change experiment parameters at all times



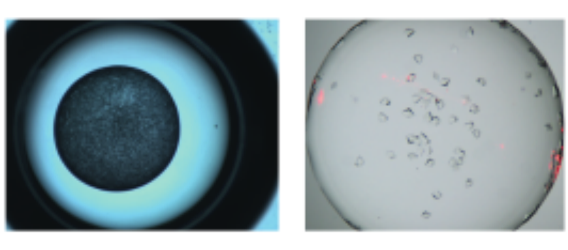
FROM INVISIBLE MOLECULAR ASSEMBLY TO MILLIMETER SIZE CRYSTALS

Interactive change of the drop composition also changes the intensity and growth rate of the nuclei or liquid clusters. Simultaneous monitoring via DLS allows to tune such events to less intensity and hence less concentrated nuclei for fewer but lager crystals.

- Dynamic access to the nucleation process in order to pre-define the outcome of the experiment
- Controlled crystal surface dissolving in order to reduce lattice defects and for maintaining crystal growth

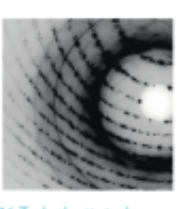
OPTIMIZATION

The ratio and quantity makes the difference that even little promising screening outcomes can be turned in to suitable crystals

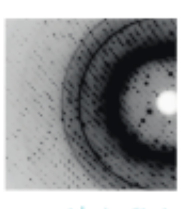


CRYOPROTECTION

Pico titration of low concentrated cryoprotectant and over 48 h by simultaneously controlled water removal increases diffraction qualaity significantly



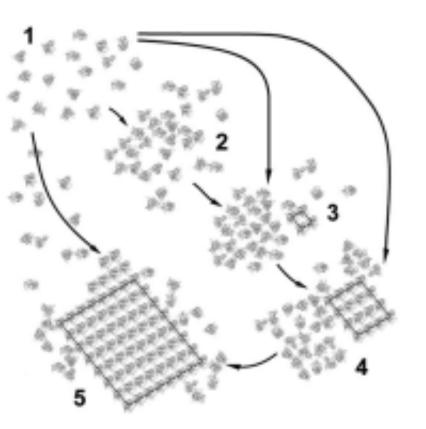
16 Tesla, levitated grown crystal , standardized applied cryo protectant, 1.4 A, high mosaicity

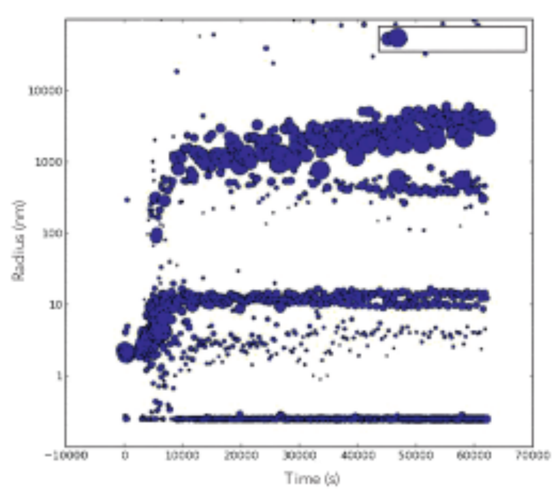


1 g grown crystal, pico titrated cryo protectant, 1.1 A, very low mosaicity

Interpretation of the Nucleation DLS Signature

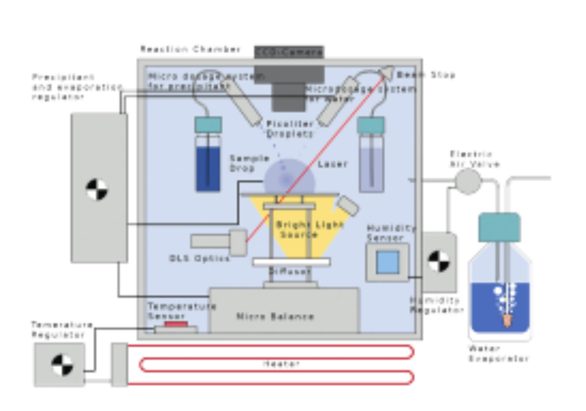
Crystallization in its very essence means to provide conditions that small particles assemble themselves to larger objects. In contrast to amorphous aggregation there's a delicate energetic situation avoiding kinetic traps leading to random oriented binding, finally resulting in an energetically favorite crystallic ordered solid state. These differences can be distingued via DLS.





The Interactive Crystallization Set-up

Piezo driven microdosage systems, micro balance and in situ DLS are the key components of this set-up. An enclosing temperature and humidity controlled chamber is essential as well.



- Fully automated experiment conduction
- Intervention possiblities at all times
- Quick Comparison with previously conducted Experiments
- Qualitative and Quantitative Output of size distribution and drop composition (+/- 2% accuracy)
- SQL-database data Management

Neutron Diffraction ✓ | Microcrystals for SFX ✓ | Nanocrystals for Micro-ED ✓

Ligand Soaking ✓ | Cryoprotection ✓ | Crystal Crosslinking ✓

XtalController 900

TECHNICAL DATA

Micro balance	Resolution 1 µg
Illumination	Bright field illumination with LED
Climate chamber	Regulated relative humidity up to 100% with a precision better than 0.1% Control of the temperature max 10°C above or below ambient, stability better than 0.1°C
Microscope	Objective: Planachromat 1x Five different magnification steps: 0.32x, 0.63x, 1x, 1.6x, 3.2x Resolution: 9.2, 4.6, 2.9, 1.8, 0.9 µm/pixel, motorized drop position setting Zoom and focus setting fully motorized
Camera	CCD color camera with a resolution of 1600 x 1400 pixel
DLS system	Laser diode wavelength/optical power: 660nm/120mW (adjustable) Measurement position in drop adjustable with computer control Detector Photomultiplier tube, dark count rate < 300 kHz Single photon counter, quantum efficiency 5-7%, count sensitivity 1.5 105 Hz/pW Fixed scattering angle for back scattering (148°) Correlator multi-tau architecture correlator with 210 quasi logarithmically spaced channels enabling sample times of 400 ns to 13.43 s sample rates Sensitivity Sample concentration with standard laser parameters Minimum concentration: 0.3 mg/ml for a 15 kDa protein, 0.1 mg/ml for a 50 kDa protein. Max. concentration ~120 mg/ml
Microdispensing system	Piezo operated drop generator for contact free addition of liquids Dispensed volume per piezo stroke: 30 pL Options for additional drop generators (e.g ligand, seeding, additives) Regulated dispensing frequencies for pre-defined time dependent sample composition.
Instrument	Table top System 650 mm x 550 mm x 450mm (LxBxH) Weight: approx. 30 kg Power consumption: 90 to 264 V 200 W Clean pressurized air 2-6 bar, oil free is required
Instrument table	For optimal performance a vibration damped table is required
Computer	Mini-PC ready to use OpenSUSE Linux Leap 15.3 Desktop PC ready to use LCD-Display 4K
Software features	Xtal-Controller software runs on Linux Determination of crystal size for control of growth rate Fully automated operation mode Full remote control via internet Integrated SQL-data base Real time monitoring of the sample composition Recording of sample composition history Live display of camera images Storage and retrieval of all relevant information in the data base

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