Crystal Growth Simulation Software

Generic Monte Carlo crystal-growth software for simulation of crystal habit and nanoscale surface topography.

www.CrystalGrower.org

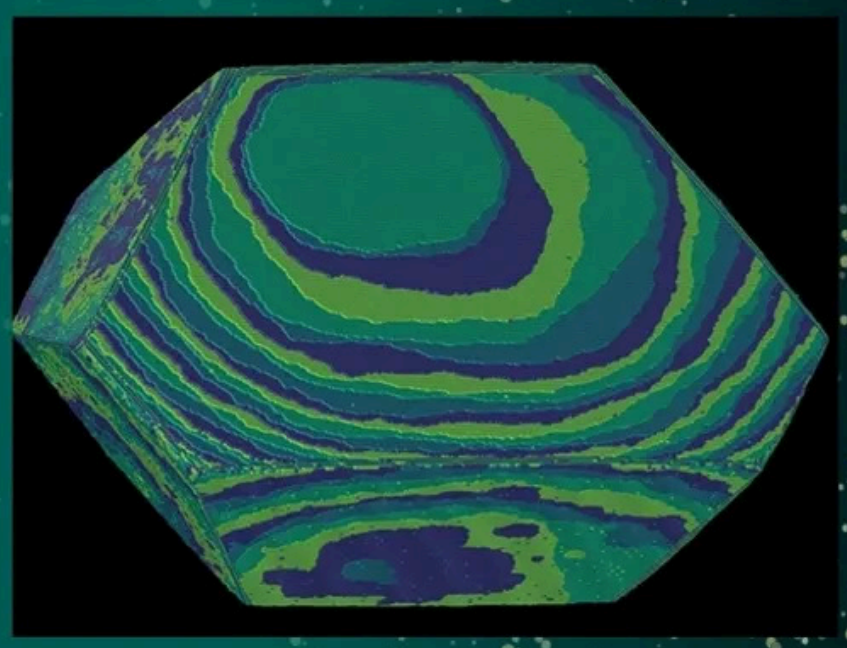
CrystalGrower

Reimagining Crystallisation, Driving Innovation

Introducing CrystalGrower

Understanding the molecular-scale growth of crystals is **crucial for optimising their performance and functionality**. With advancements in scanning-probe microscopy, we can now access detailed molecular surface topography data. **When combined with measured crystal habits, this provides a wealth of experimental insights essential for enhancing our understanding** and gaining deeper insights into crystal growth dynamics. Our software is tailored to extract and leverage this information effectively, empowering you to **maximise your understanding of your crystal system's behaviour** and customise crystallisation conditions accordingly.

2021 HORIZON PRIZE



New software to simulate crystal growth

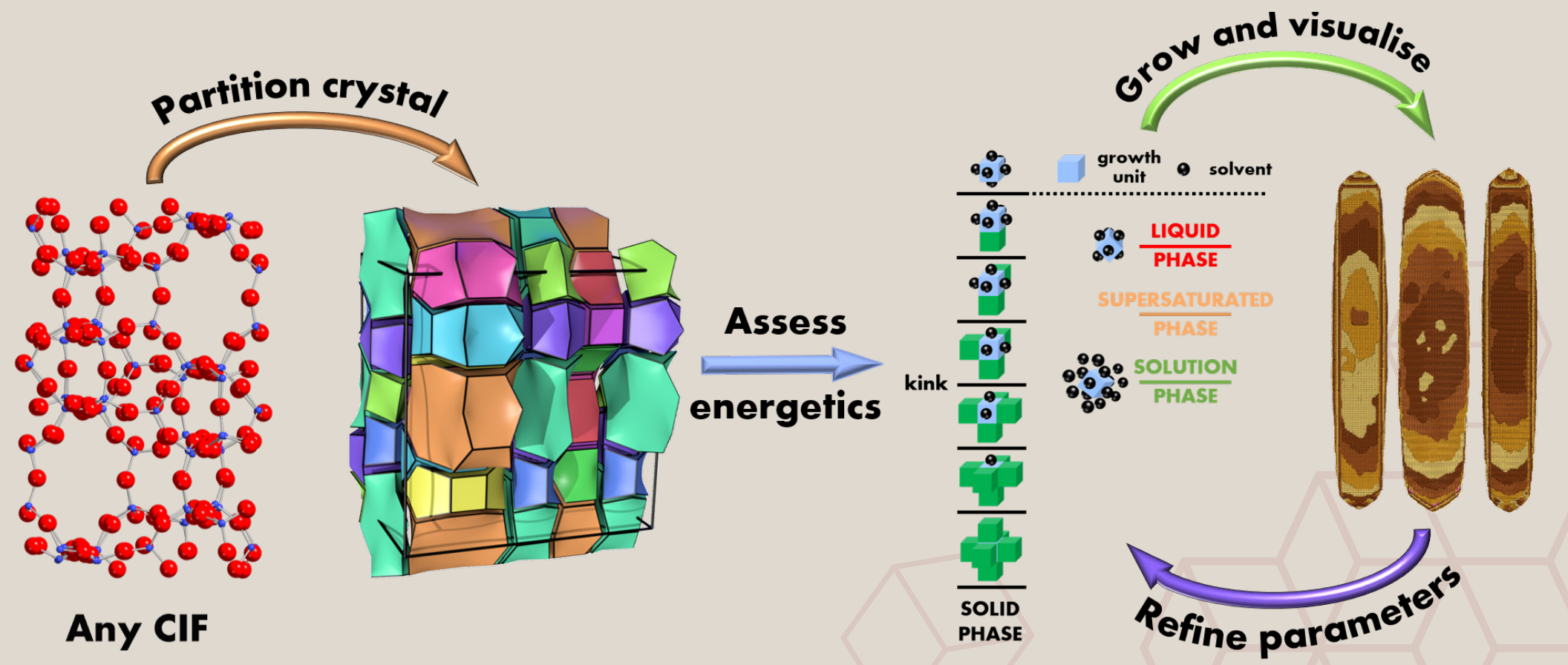
Materials Chemistry Division
Horizon Prize:
Stephanie L Kwolek Award

#RSCPrizes

ROYAL SOCIETY OF CHEMISTRY

How do we do it?

Starting from crystallographic information files (CIFs), our software offers deep insights into crystal habit and nanoscale surface topography. **Incorporating Monte Carlo predictions and a thorough understanding of the free energies of crystallisation** within your crystal structure, we predict how your crystals grow by identifying the sites most likely to undergo growth or dissolution. This generic approach seamlessly **merges the thermodynamics of crystal growth with the crystallography** of your system.



Curious to learn more about our methodologies? Scan the QR codes below to explore the research papers that define CrystalGrower.

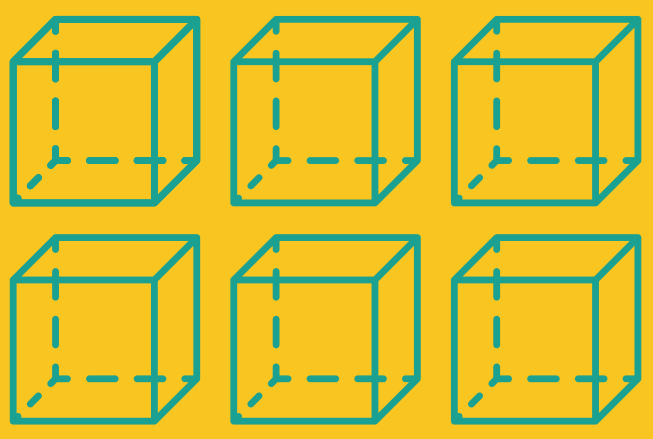
Industry

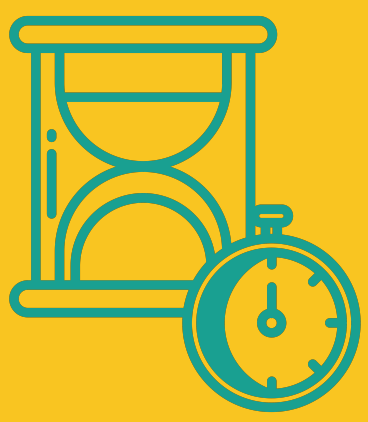
What we can do for you:

Increase cost savings
Maximise cost savings by implementing more efficient crystal growth processes, minimising waste and optimising resource utilisation.

Optimise morphologies for industrial applications
Tailor crystal morphologies to meet specific industrial requirements, improving product performance.

Improve product quality and consistency
Minimise defects and variability in production batches by enhancing the uniformity and quality of crystalline products, ensuring consistent product reliability.





Accelerate research and experimental efficiency
Optimise research processes to accelerate development cycles, alleviate workforce demands, and expedite time-to-market for products.

Benefit from our research collaborations
We collaborate with top research institutions to advance the understanding of crystallisation, ensuring that our software remains at the forefront of industry advancements.

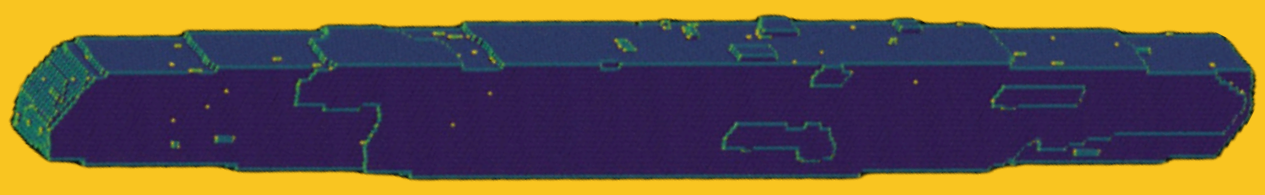
Make your research sustainable

Perform solvent screening computationally by evaluating 180 solvents, you can select greener solvent alternatives.

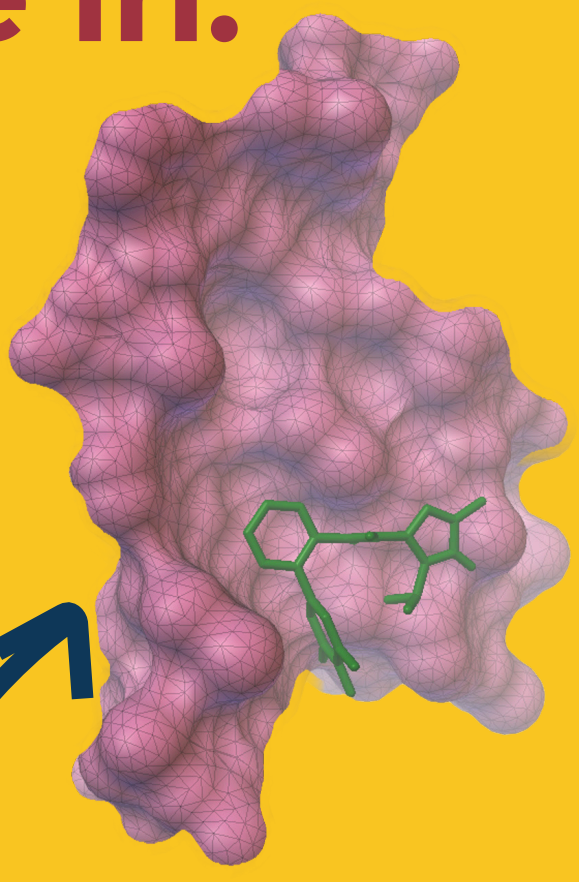
Applications

Sectors we operate in:

Pharma



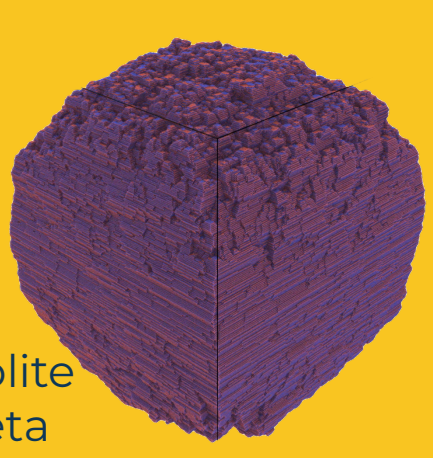
Crystal*Grower* can better control crystal size and shape, to improve the solubility and bioavailability of drugs. This leads to more consistent therapeutic outcomes and improved patient compliance.

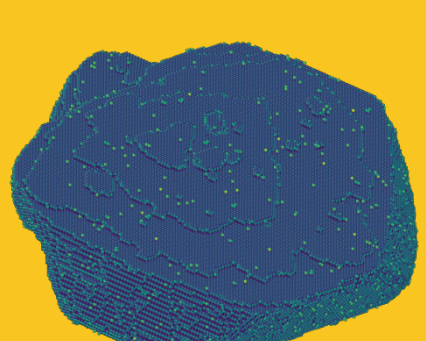


Food

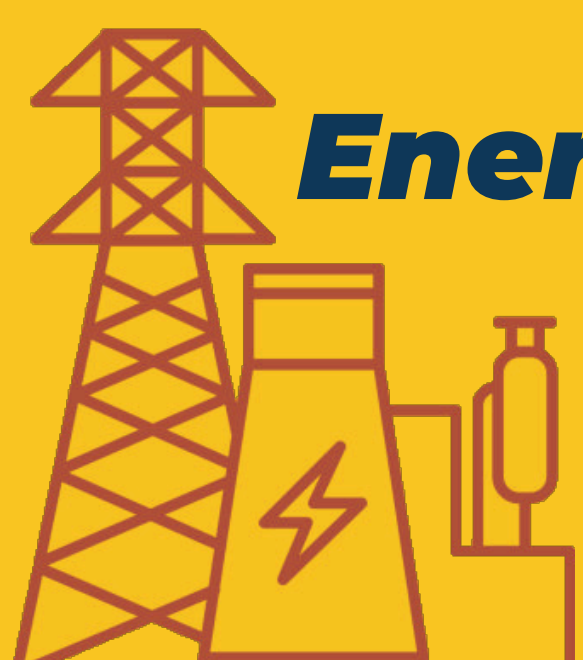
Agrochemical

Technology





Energy



Crystal*Grower* can be used to improve energy density and stability in battery materials. Resulting in longer lifespans, faster charging times, and higher efficiency.

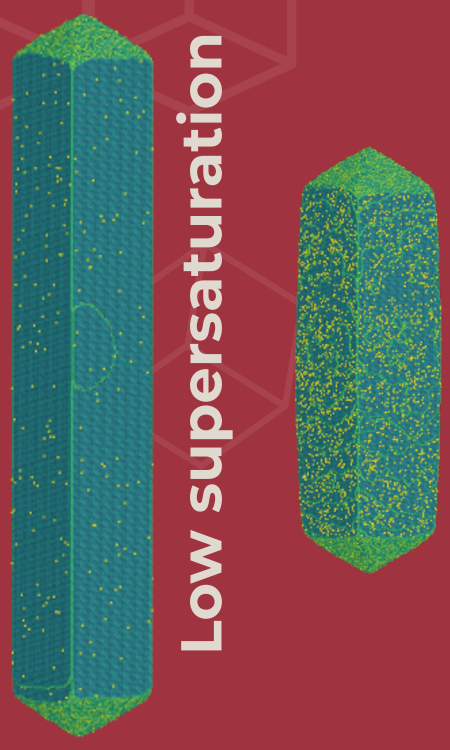
Mining

Academics

Download our free academic version here

Features you

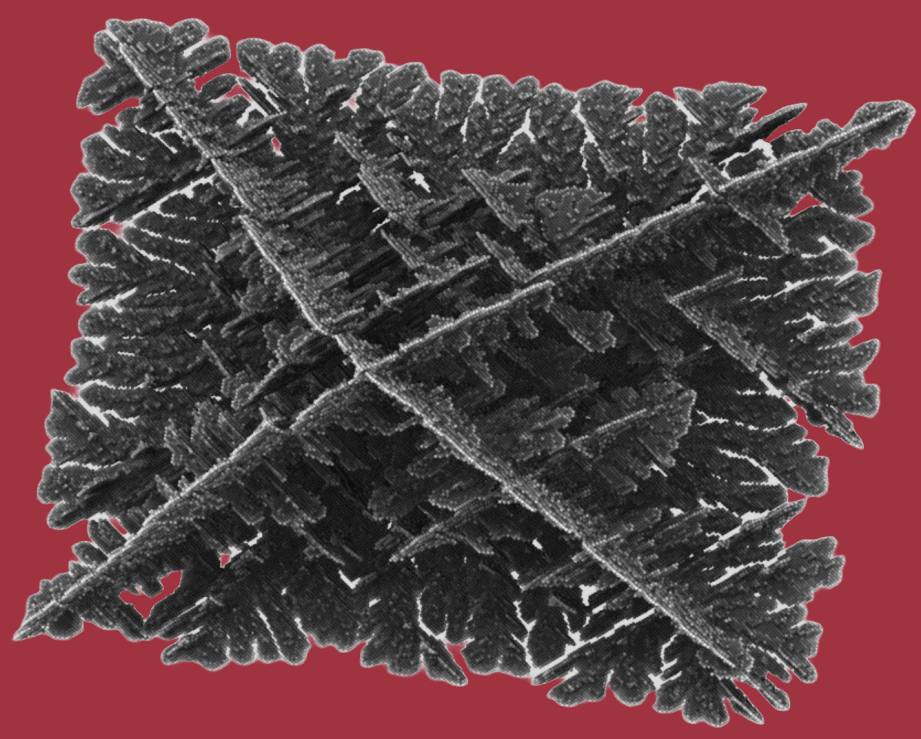
Supersaturation



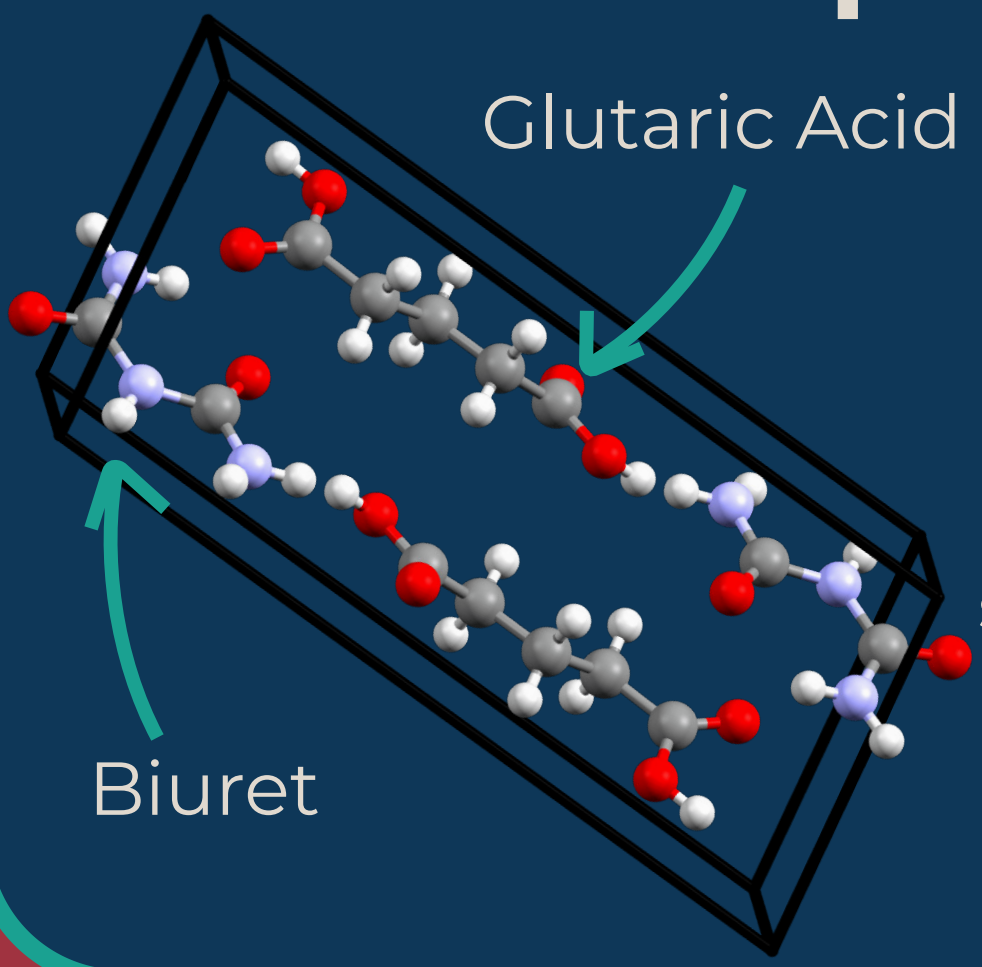
We can predict the effects on morphology under various supersaturation conditions, through detailed simulations. This approach enables precise analysis of surface energies.

Diffusion

By varying local supersaturation values, we can model complex growth regimes such as diffusion-controlled and dendritic growth



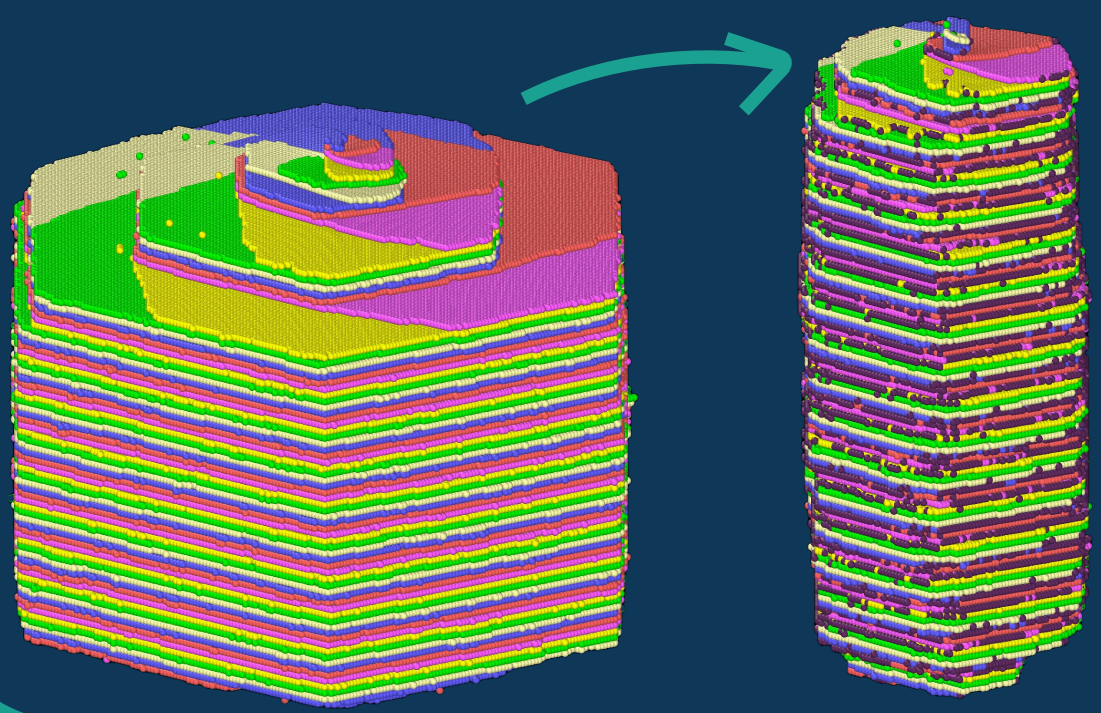
Multicomponent systems



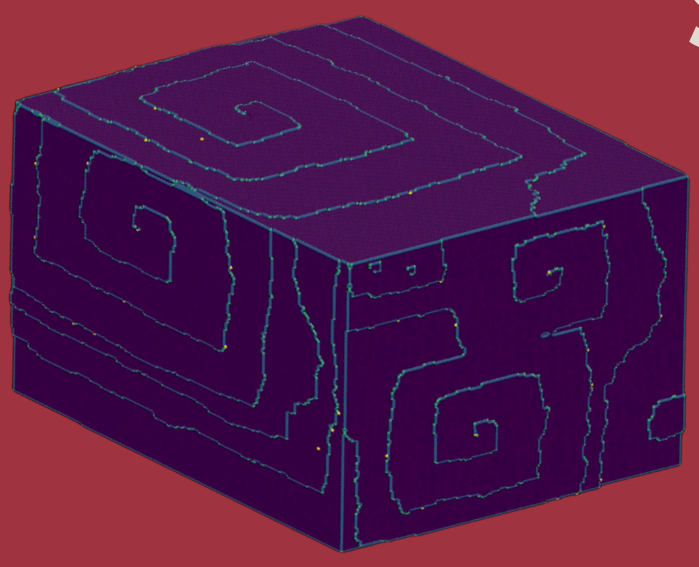
Investigate the influence of individual components on crystallisation within multicomponent systems by adjusting their relative concentrations in both solution and solid states. Study both ordered cocrystals and complex disordered systems, such as solid solutions.

can analyse

Growth Modifers



Model the impact of growth modifiers on crystal morphologies by simulating their attachment to sites within the crystal lattice.

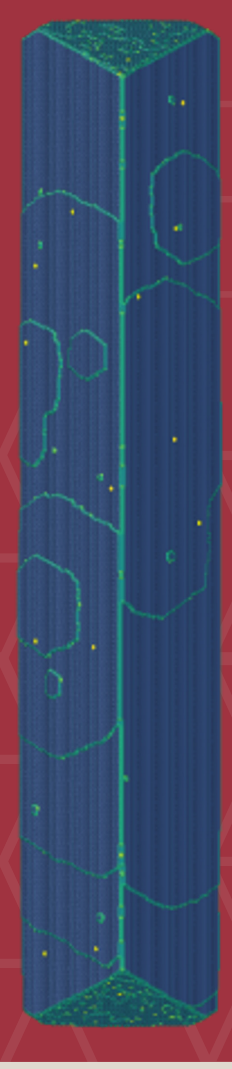


Screw dislocations

Model families of screw dislocations, which dramatically alter relative crystal growth rates by removing 2D nucleation barriers.

Temperature Cycling

Adjust temperature and supersaturation profiles throughout the crystal growth simulation to understand how experimental conditions change crystal features and morphologies.



And this is just the beginning! Discover even more features on our website. Visit us at www.CrystalGrower.org to learn more.

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