Simulating Crystal Growth with Contaminant Diffusion

Computational Analysis in MATLAB

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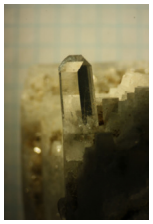

Crystal image taken from Canton Ticino, Switzerland

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Introduction

Radiometric dating is one of the most popular methods of exploring the history of Earth, but not all environments have reliable radioactive isotopes. Diffusion profiles of crystals contain information on the state of the environment at different times in the crystal's lifespan, and this analysis is the foundation of examining diffusion profiles. This allows us to better understand the evolution of fluid flow in geological environments, in which many of our resources come from.

Anatomy of a Crystal

A crystal grows by adding new silica layers on the crystal's top faces. The faces attract molecules from the surrounding fluid to become part of the new growth, and is mostly composed of silica plus a small amount of contaminants. The contaminants are able to diffuse out of the crystal, and this diffusion is regulated by variables such as time and temperature. These variables can be analyzed in a diffusion profile. The concentration of contaminants can be found by solving for this differential equation, which is shown in the Finite Difference Method section below.

$$\frac{\partial C}{\partial t} = k_x \frac{\partial^2 C}{\partial x^2} + k_z \frac{\partial^2 C}{\partial z^2}$$

Variables Involved

The rates of diffusivity in the two dimensions are the variables k_x and k_z, and are inherent to the specific crystal. In quartz, diffusion out the top occurs approximately ten times faster than diffusion out the side; $k_z = 10\,k_x$.

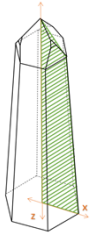
The level of contaminants that are added to the new growth of the crystal is determined by the surrounding fluid. This is implemented into the program by adding a specified amount of contaminants onto every growth, and through diffusion this growth is leveled off to be uniform with the rest of the crystal.

Programming in MATLAB

Assumptions

This analysis omits the third dimension and instead looks at a 2-dimensional vertical slice of a crystal. This allows us to use the axial symmetry of the crystal in order to simplify the computation.

The current programs grow and diffuse the crystal at a constant rate, assuming no changes in the external environment. In reality, temperature and contaminant changes will alter the growth and diffusion rates.



Spatial dimensions *x* and *z*

Finite Difference Method of Solving PDE's

Two-dimensional diffusion is modeled with the partial differential equation

$$\frac{\partial C}{\partial t} = k_x \frac{\partial^2 C}{\partial x^2} + k_z \frac{\partial^2 C}{\partial z^2}$$

where *C* is the function of concentration of contaminants at one instant in time, and k_x and k_z are the diffusivity constants for the respective dimensions. Using the numerical method of finite differences for solving partial differential equations, the result is

$$\frac{{C_{i,j}}^{n+1} - {C_{i,j}}^{n}}{\Delta t} = k_x \frac{{C_{i,j+1}}^{n} - 2{C_{i,j}}^{n} + {C_{i,j-1}}^{n}}{(\Delta x)^2} + k_z \frac{{C_{i+1,j}}^{n} - 2{C_{i,j}}^{n} + {C_{i-1,j}}^{n}}{(\Delta z)^2}$$

Where *i* and *j* represent positions in *x* and *z*, respectively, and *n* is the time index. This can be solved for the future timestep:

$${C_{i,j}}^{n+1} = {C_{i,j}}^{n} + s_x\left({C_{i,j+1}}^{n} - 2{C_{i,j}}^{n} + {C_{i,j-1}}^{n}\right) + s_z\left({C_{i+1,j}}^{n} - 2{C_{i,j}}^{n} + {C_{i-1,j}}^{n}\right)$$

Where $s_x = \frac{k_x \Delta t}{(\Delta x)^2}$ and $s_z = \frac{k_z \Delta t}{(\Delta z)^2}$

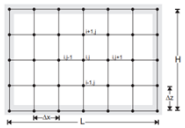
This calculation is applied to every element of the current crystal matrix at time *n* to determine the approximate value of contaminants per element for the future crystal matrix at time *n+1*.

Courant Condition

The Courant Condition, which restricts the values of s_x and s_z, is a limit on the size of the spatial steps Δx and Δz, and time steps Δt. A Courant Condition that is too large results in unstable solutions, so for our simulation a value of 0.1 was appropriate. Selecting the Courant Condition dictates the change in time per diffusion iteration, Δt.

Boundary Conditions

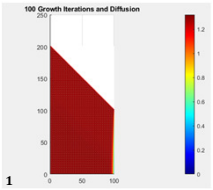
No diffusion occurs on the bottom and left edges due to direct contact with the rock face and axial symmetry. In the model, diffusion out the sides can be prevented by adding a temporary layer next to the left side and the bottom whose values are equal to the original edges, making the gradient between the two zero.



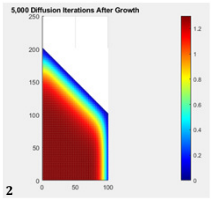
Finite difference for one position; *i,j*

Diffusion Over Time

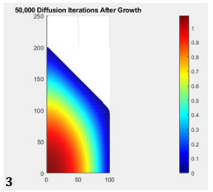
$k_x = 1; k_z = 10$



1 Initial Crystal, Step 1

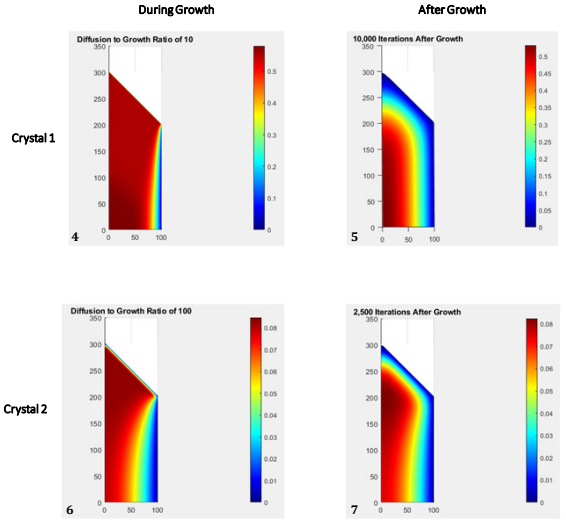


2 Short Timespan, Step 2



3 Long Timespan, Step 3

Changing Diffusion-to-Growth Ratio



The color scales correspond to the value of contaminants, the function *C*, at each position in an instant of time. Note that the color scales are independent for each graph.

Conclusion

Modeling Crystal Behavior

The diffusion profiles above resemble actual diffusion profiles measured in naturally grown crystals.

During growth, diffusion does not occur out the top face. The initial layer added with the set value of contaminants does diffuse, but eventually levels out at a value that is dependent on the speed of the growth. This can be shown in Graph 1, as there is no gradient on the top face.

Crystals 1 and 2 show the contrast between fast and slow growth, and how more diffusion occurs during slow growth, but diffusion out the top is still restrained until growth has stopped.

Graphs 1,2, and 2 show the relationship between diffusivities k_x and k_z. Diffusion in the *z* direction is ten times faster than diffusion in the *x* direction, which is evident in Graph 2.

Future Ambitions

The next stage of research involves updating this simulation to consider more real-life variables, such as:

- A 3-dimensional structure with diffusion in every direction
- Allowing the diffusion and growth rates to change during simulation to better reflect real crystal growth.

The ultimate goal is to compare the final model's simulated diffusion profiles to naturally-grown crystal profiles to gain insight on environments in which natural crystals grow.

Sources and Acknowledgments

Becker, Thorsten; Kaus, Boris. *Numerical Modeling of Earth Systems.* March 8th, 2016.

Brinza, E.M., Fitzpatrick, W.A., and Ihinger, P.D. (2017) The Distribution of Hydroxyl Species in Hydrothermal Quartz Crystals: The Dominant Role of Post-Crystallization Diffusion, *Geological Society of America Abstracts with Programs*, Vol. 49, No. 6, *Paper #172-14.*

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