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The role of grain boundary energy anisotropy on the grain size evolution during normal grain growth

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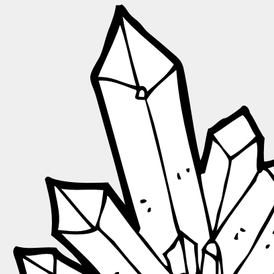
EGU European Geosciences Union



Presented by:

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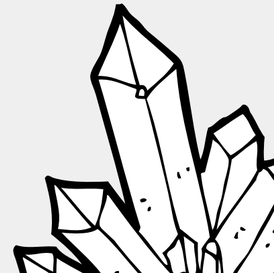
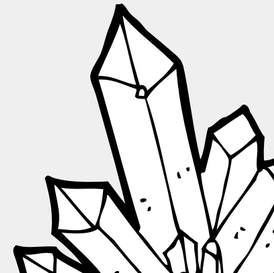


Motivation

Many regions of the Earth's mantle deform in grain size-sensitive creep regimes. The grain size right below the transition zone is believed to be very small, and the grain size should in subsequent depths be mainly controlled by normal grain growth. The grain size evolution is commonly predicted using either analytical grain growth laws in combination with grain boundary diffusion coefficients or by extrapolating empirically determined grain growth laws. Effects of Zenner pinning and different ratios of second phases have been studied, while the role of anisotropic grain boundary properties is mostly neglected

The grain boundary energy varies with the orientation of the grain boundary plane, as expressed through the typical crystal habitae (Wulff-shapes). Individual crystals in a polycrystalline material maintain a grain boundary energy anisotropy during grain growth.



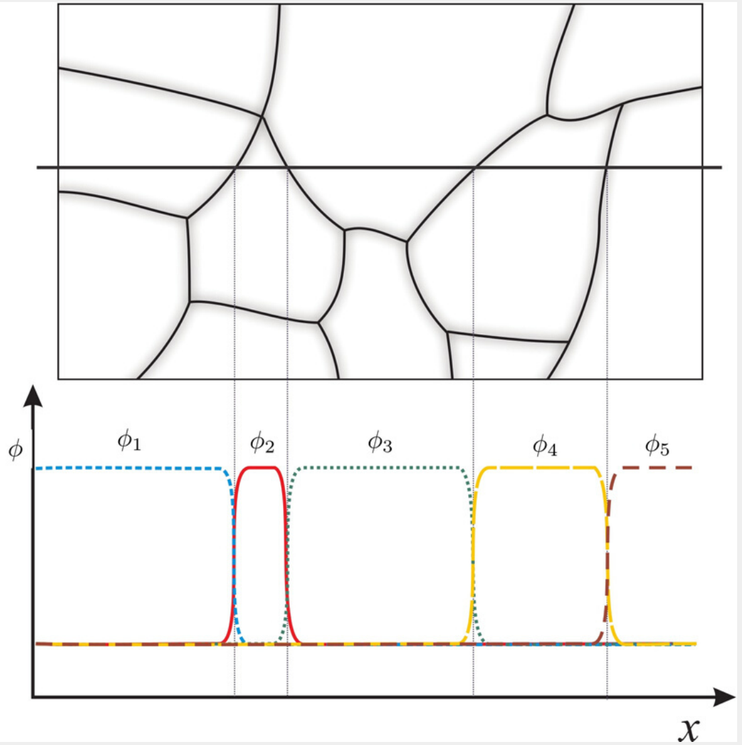
The aim

Here we study, how grain boundary anisotropy impacts grain boundary migration and normal grain growth rates by three-dimensional phase-field simulations. We imply grain boundary energy minimization by faceting the grain boundary i.e. varying the grain boundary planes to minimize the grain boundary energy. The grain boundary energy anisotropy for the solid-solid interface is taken from experimentally investigated grain boundary plane distributions and grain boundary energy distributions on periclase (MgO). We compare the grain size evolution in simulations with isotropic and anisotropic grain boundary energy of cubic crystal symmetry.

The Method

Phase-Field Method

The phase-field method is a mathematical model for solving interfacial problems. It is increasingly applied as a robust numerical method to study materials with numerous types of microstructure evolution processes. These include phase transformation, solidification, grain growth, dislocation-solute interactions and multicomponent interdiffusion.



The time evolution equation of the phase-field parameter is constructed as a sum over all dual interactions between the grains :

$$\dot{\phi}_\alpha = -\frac{\pi^2}{8\eta}\sum_{\beta=1}^{N}\frac{\mu_{\alpha\beta}}{N}\left(\frac{\delta F}{\delta\phi_\alpha}-\frac{\delta F}{\delta\phi_\beta}\right)$$

The grain boundary energy is given by :

$$f^{GB} = \sum_{\alpha\neq\beta}^{N}\left[-\frac{4\eta\sigma_{\alpha\beta}}{\pi^2}\nabla\phi_\alpha\cdot\nabla\phi_\beta+\frac{4\sigma_{\alpha\beta}}{\eta}\phi_\alpha\phi_\beta+\sum_{\gamma\neq\alpha,\beta}^{N}\frac{8\sigma_{\alpha\beta\gamma}}{\eta}\phi_\alpha\phi_\beta\phi_\gamma\right]$$

Steinbach, I., 2009

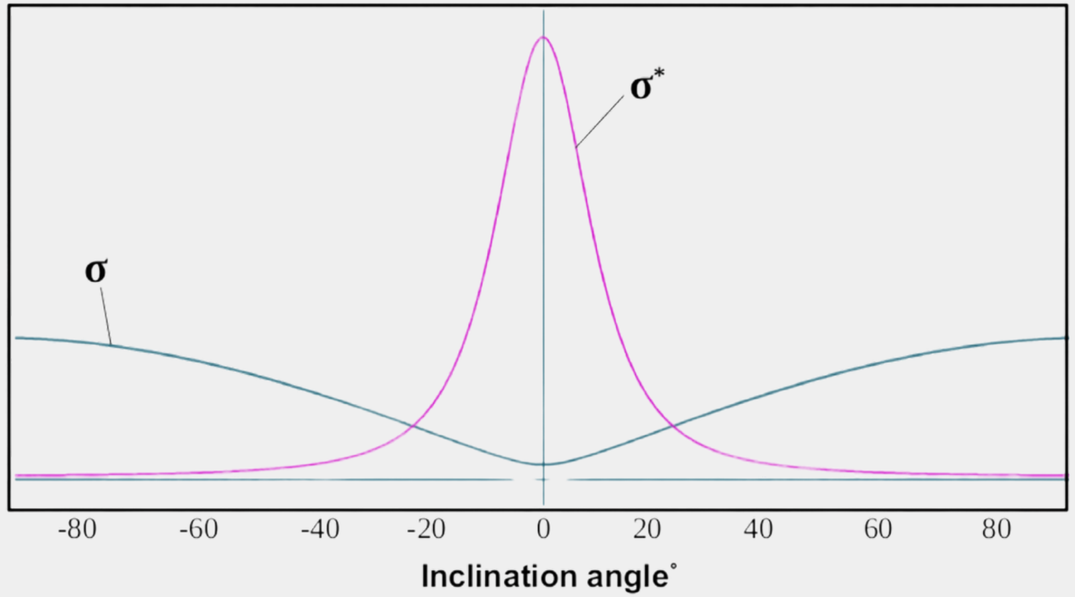
Anisotropic grain boundary energy (Faceted Model)

The kinetic equation of the phasefield reads:

$$\dot{\phi}_\alpha = \sum_{\beta\neq\alpha}^{N} \frac{\mu_{\alpha\beta}}{N} \left\{ \sum_{\gamma\neq\alpha,\beta}^{N} \left[\sigma^*_{\beta\gamma} - \sigma^*_{\alpha\gamma}\right] \left[\nabla^2\phi_\gamma + \frac{\pi^2}{\eta^2}\phi_\gamma \right] + \sum_{\delta\neq\gamma}^{N} \frac{\pi^2}{\eta^2} \left[\sigma^*_{\alpha\gamma\delta} - \sigma^*_{\beta\gamma\delta}\right] \phi_\gamma\phi_\delta + \frac{\pi}{\eta}\sqrt{\phi_\alpha\phi_\beta}\,\Delta G_{\alpha\beta} \right\}$$

σ^* is the interface stiffness which is given by :

$$\sigma^*_\alpha = \sigma_\alpha(\theta_\alpha) + \sigma''(\theta_\alpha) = \frac{\sigma^0 a^2}{\left(\sin^2(\theta_\alpha) + a^2\cos^2(\theta_\alpha)\right)^{\frac{3}{2}}}$$



The energy of a solid-amorphous interface is calculated as :

$$\sigma_\alpha(\theta_\alpha) = \sigma^0\sqrt{\sin^2(\theta_\alpha) + a^2\cos^2(\theta_\alpha)}$$

Steinbach, I., 2009

The Code

All the results have been simulated using the open source library OpenPhase.

OpenPhase
Solutions GmbH

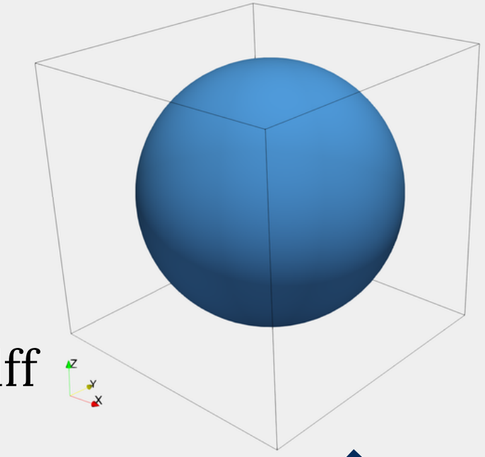
About OpenPhase:

OpenPhase is the open source software project targeted at the phase-field simulations of complex scientific problems involving microstructure formation in systems undergoing first order phase transformation. The core of the library is based on the multiphase field model. The project has the form of a library and is written in object oriented C++.

Visit the project website :

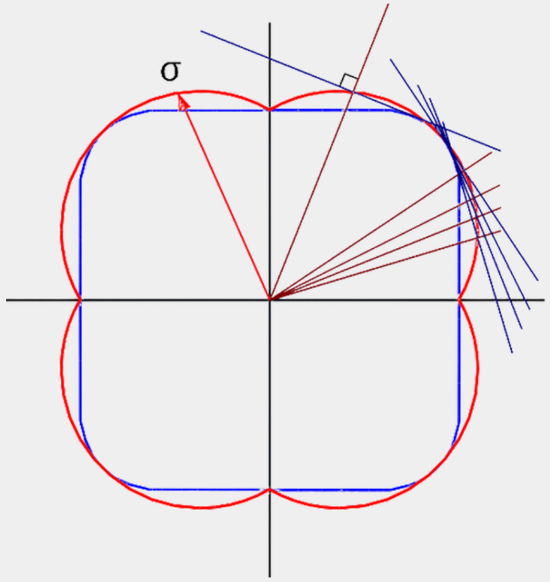
Valdiation

Equilibrium shapes

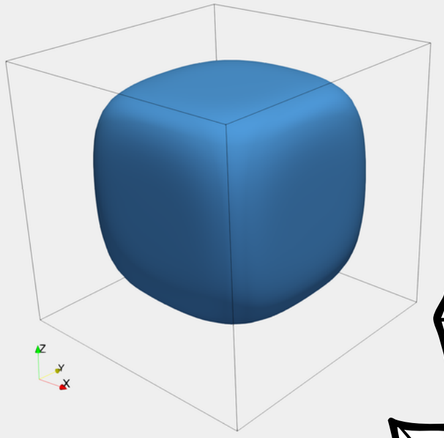


The equilibrium shape can be determined by the Wulff construction. The Wulff theorem states that a point-to-plane distance from the center of a particle to a facet is proportional to the surface energy of the facet.

The reader can watch the time evolution toward the equilibrium shape by scanning the QRcode.



As a first application of the theoretical model introduced above, the case of equilibrium shape is investigated in 3D by performing a simulation of an initially spherical grain inserted in the melt in a simulation box of size 128x128x128 grid points.



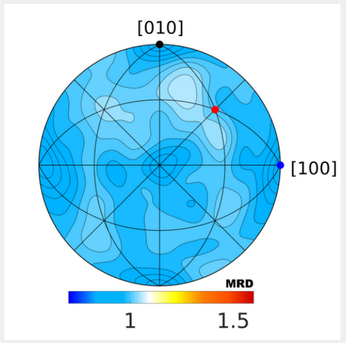
Grain Growth Simulations

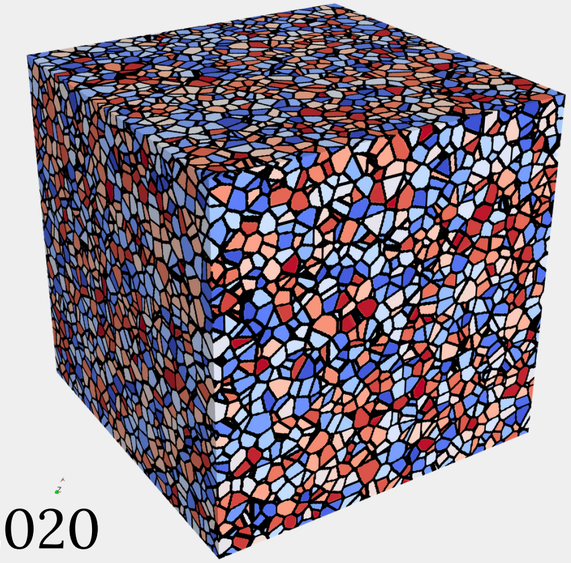
Simulation setup:

- Simulation box: 400x400x400 grid points.
- Number of grains: 18000 grains.
- Orientation: random crystallographic orientations are assigned to all grains.
- We compare two cases:
  1- Isotropic grain boundary energy
  2- Anisotropic grain boundary energy (Faceted model) -- Results shown here

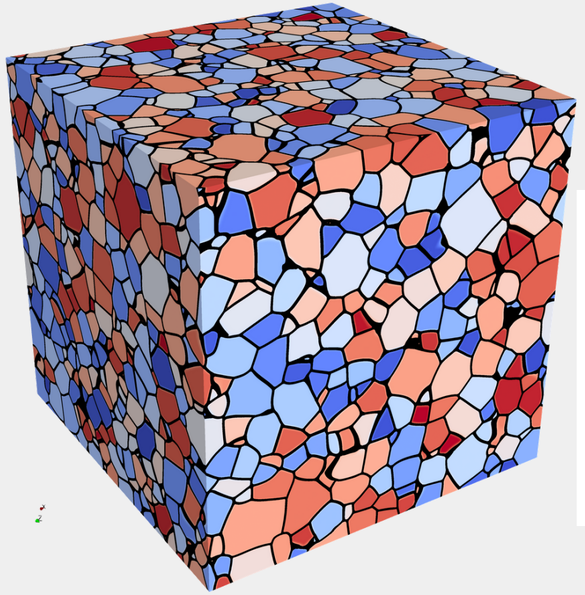
Simulation Results:

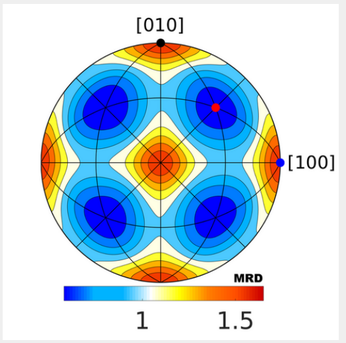
- The simulations show that the anisotropic system exhibits retardation (slowdown) in grain growth compared to the isotropic system.
- Grain boundary plane distribution has a peak toward low index {100} planes.





hint: scan the QRcode





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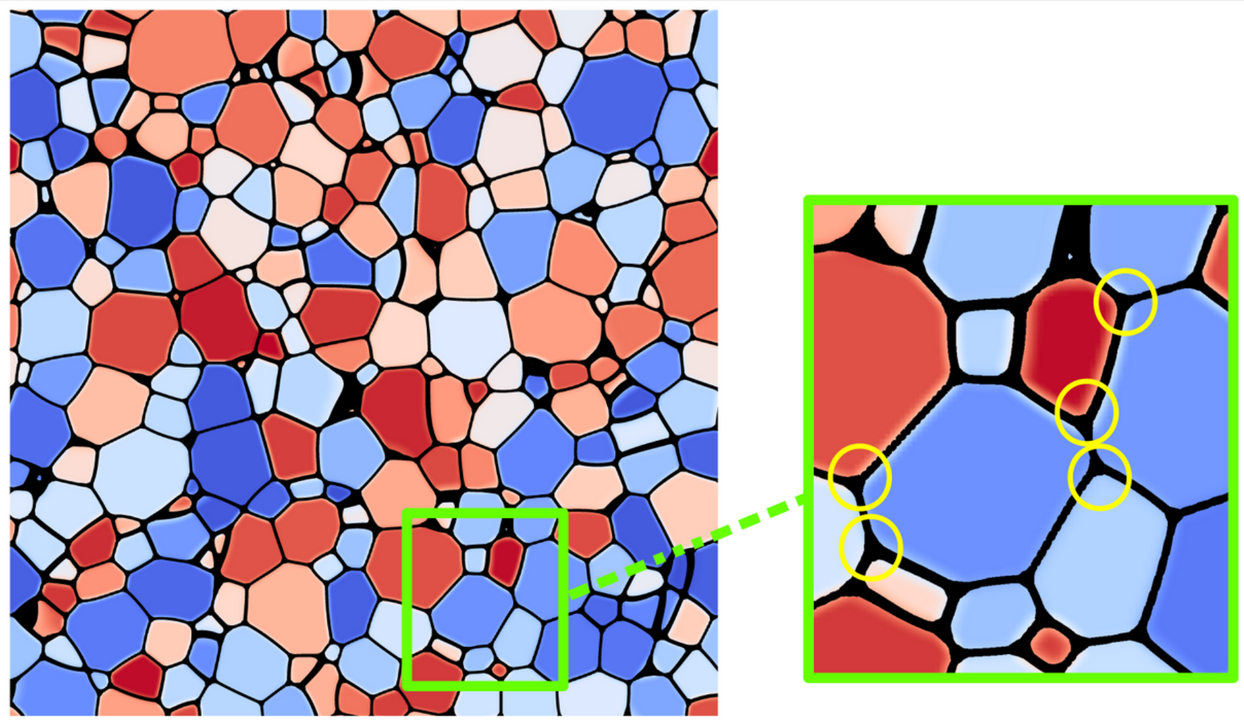
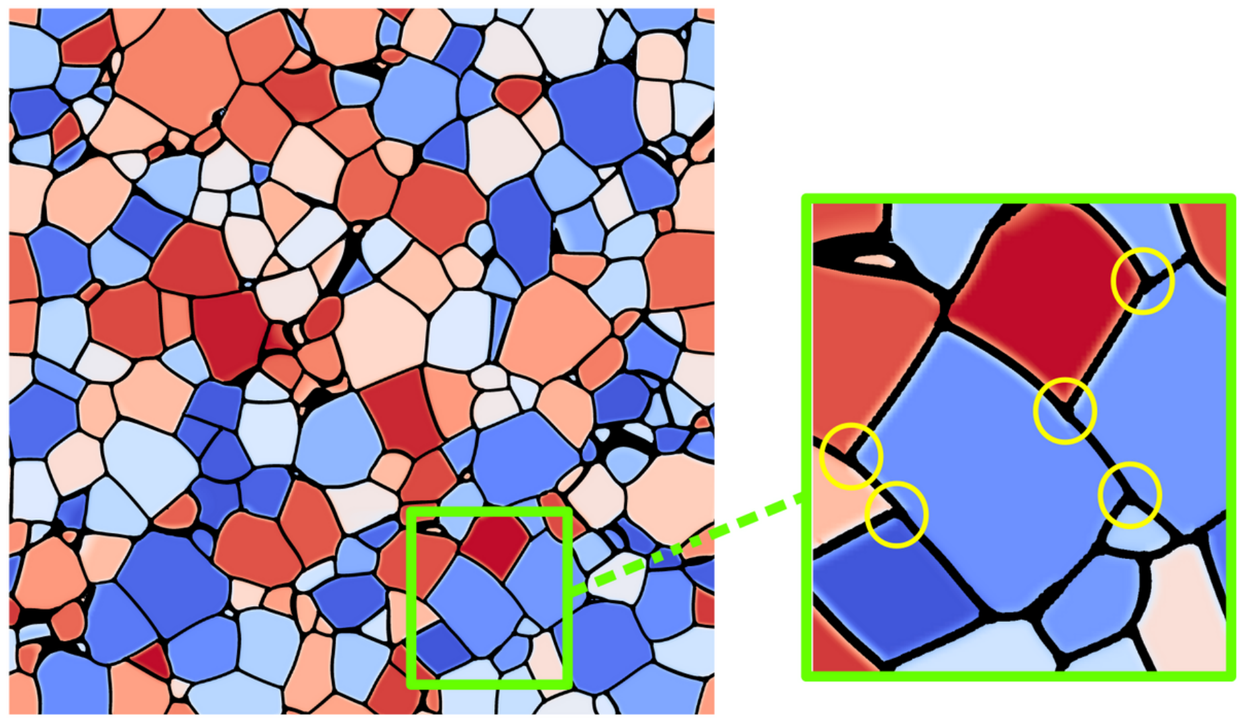
Effect of anisotropic grain boundary energy on microstructure

The microstructure exhibit the presence of more frequent triple-junction angles close to 90 and 180 degrees (marked with yellow circles) as a result of the development of faceted grains.



Isotropic grain boundary energy

Anisotropic grain boundary energy



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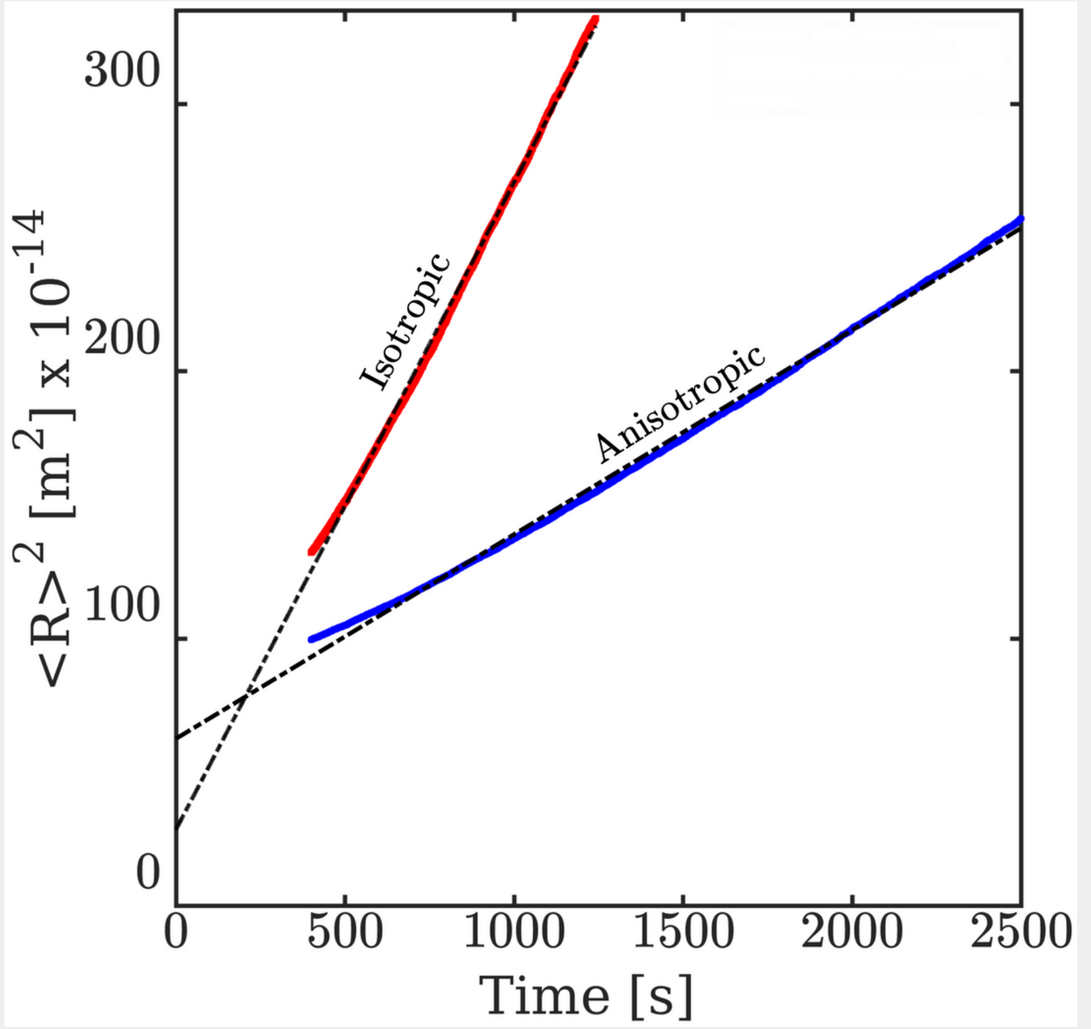
Grain Growth Rate

Growth rate of Isotropic vs Anisotropic

- Growth rate for anisotropic case is slower than that in isotropic case. This is considered to be due to the fact that the number of lower energy boundaries in anisotropic case increases with time.

- The rate of grain growth for periclase is a factor of 3 smaller compared to an isotropic material



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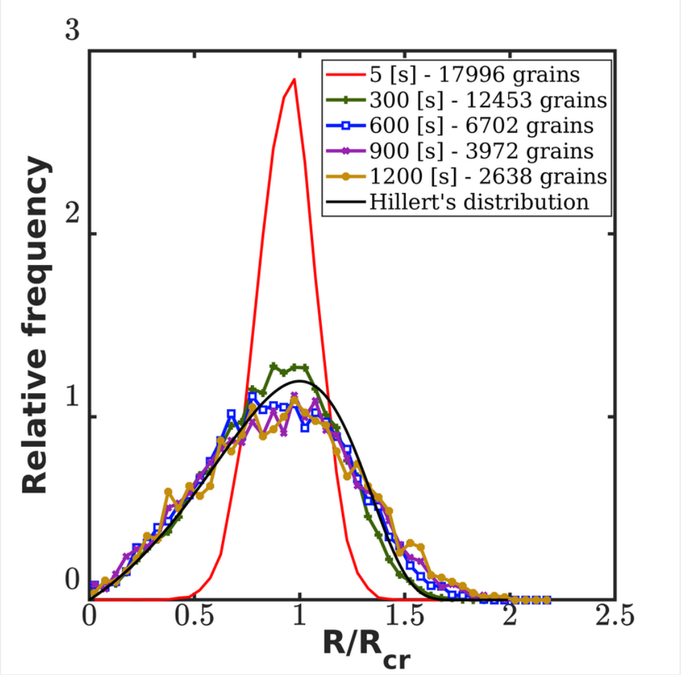
Grain Size Analysis

Comparison to mean-field theories for normal grain growth

- The grain size distribution for the isotropic case agrees with Hillert's prediction on normal grain growth.

- The simulated grain size distribution for the case of anisotropic grain boundary energy has a clear shift toward small grain sizes.



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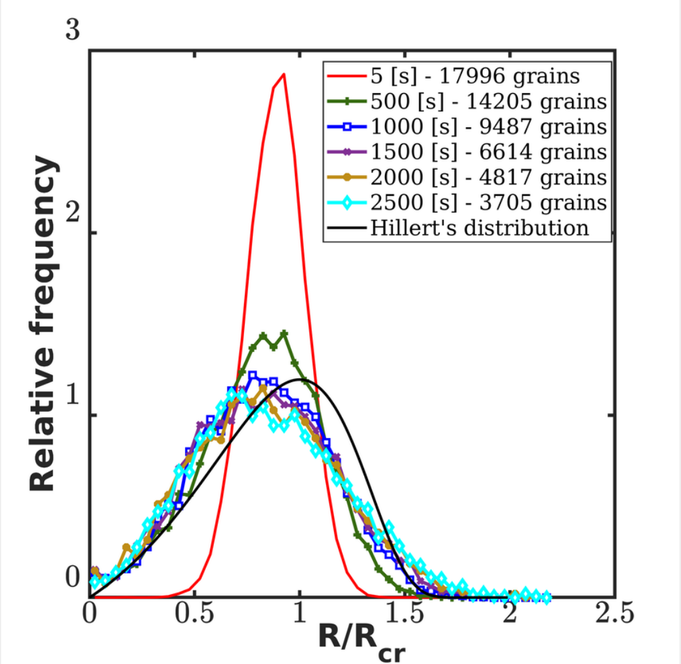
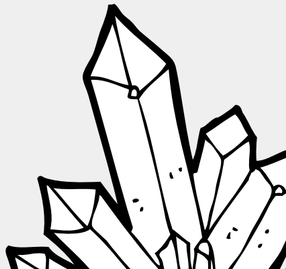


Conclusion

These results are of three-fold importance:

1. The classical theory of grain growth is developed for purely isotropic materials and thus fails to predict grain growth for materials with anisotropic grain boundary energy.
2. Predicting grain growth using existing rate-laws and grain boundary diffusion studies can lead to an incomplete conclusion and a distorted picture of the real phenomenon.
3. Because energy reduction associated with grain growth is small, already small energy variations, such as those associated with grain boundary energy anisotropy, can have a significant effect.

A better prediction of grain size evolution in real anisotropic systems requires an anisotropic theory for grain growth which also addresses the pressure effects on both grain boundary energy anisotropy and diffusion.



References

Have a look at our publication:

- *Steinbach, I., 2009. Phase-field models in materials science. Modelling and simulation in materials science and engineering, 17(7), p.073001.*

- *Salama, H., Kundin, J., Shchyglo, O., Mohles, V., Marquardt, K. and Steinbach, I., 2020. Role of inclination dependence of grain boundary energy on the microstructure evolution during grain growth. Acta Materialia.*

How to Reach Us

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Thank you!

Questions? Let’s chat!