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Growth and characterization of two-dimensional poly(quasi)crystals

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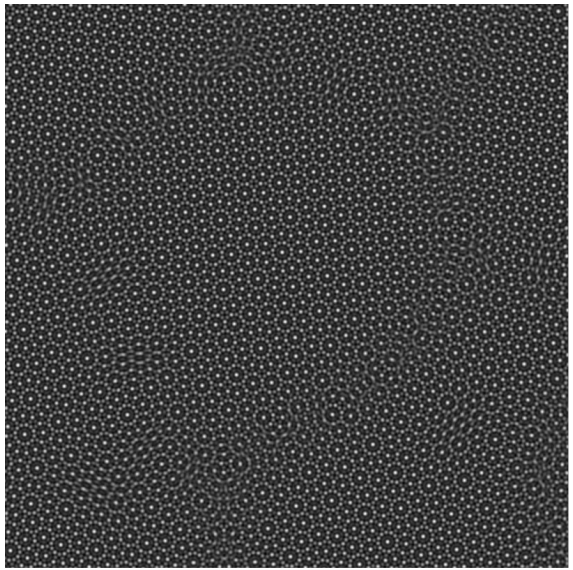
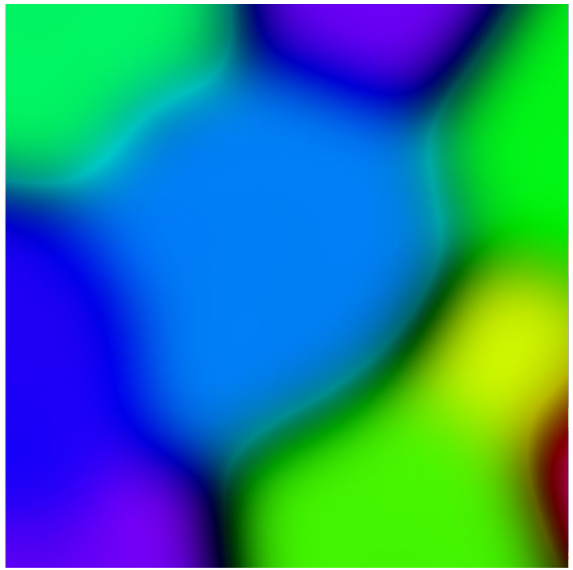
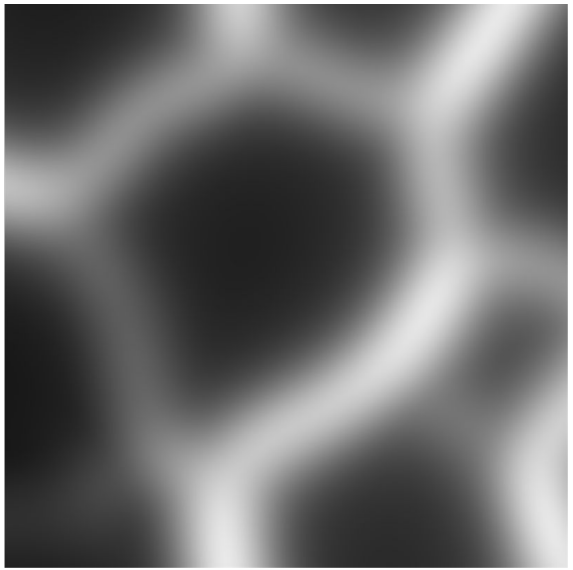

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Outline[a]

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- Motivation
- Method for characterizing (quasicrystal) microstructures
- Phase field crystal (PFC) for model system density fields
- Assessment of characterization method
- Analysis of different microstructures
- Conclusions

[a] *Hirvonen et al., Grain extraction and microstructural analysis method for two-dimensional poly and quasicrystalline solids, submitted to Phys. Rev. Materials (June 2018),* ***arXiv:1806.00700***

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Motivation

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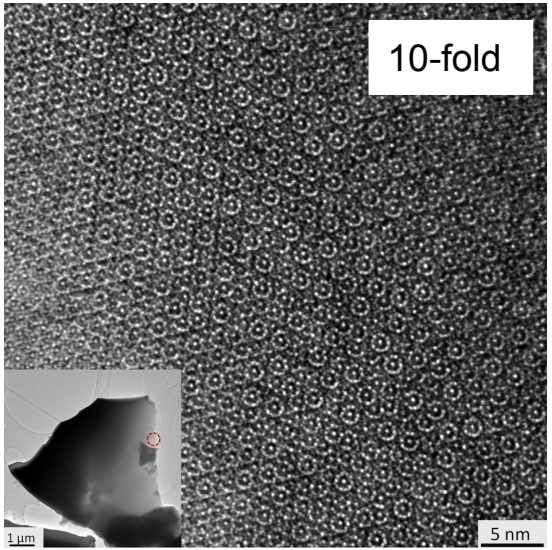
- Quasicrystals have many potential applications due to their interesting properties
  - Low μ, resistance to oxidation[a], etc.[b, c]
- Microstructure → material properties
  - What are the connections?
  - Modeling microstructures very difficult
- Quasicrystals' aperiodic nature
  - Characterization difficult



Bindi et al., Sci. Rep. ***5*** *(2015)*

[a] *Thiel, Annu. Rev. Phys. Chem.* ***59*** *(2008)*
[b] *McGrath et al., J. Phys. Condens. Matt.* ***14*** *(2002)*
[c] *Smerdon et al., J. Phys. Condens. Matt* ***20*** *(2008)*

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Grain extraction method

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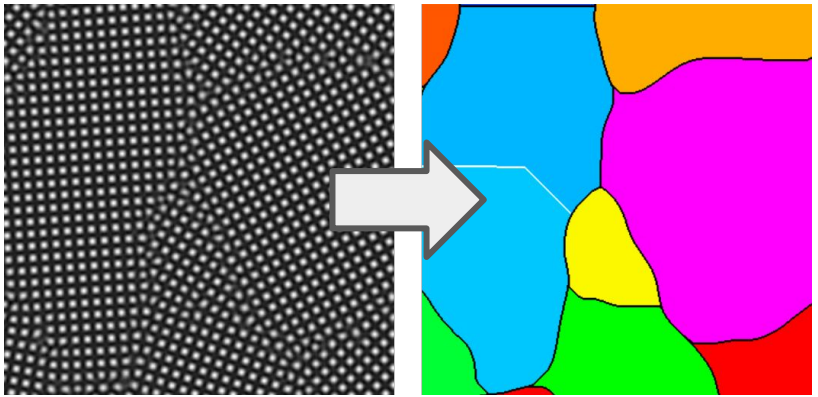
- A new **highly generalizable** method for grain extraction
  - Find grains → study microstructural properties and their distributions
  - Works for many lattice types --- **also for quasicrystals**!
- Four-step algorithm for grain extraction from atomic density maps
  1. Generate orientation field
  2. Generate deformation field
  3. Grow subdomains in deformation field
  4. Merge subdomains



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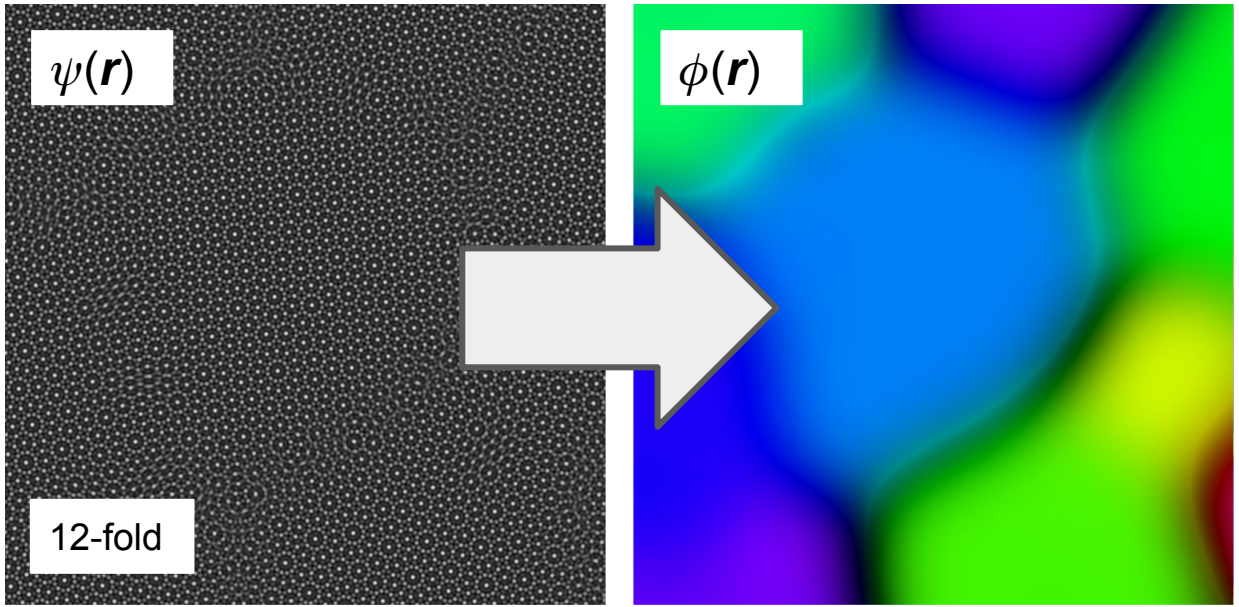
Grain extraction method

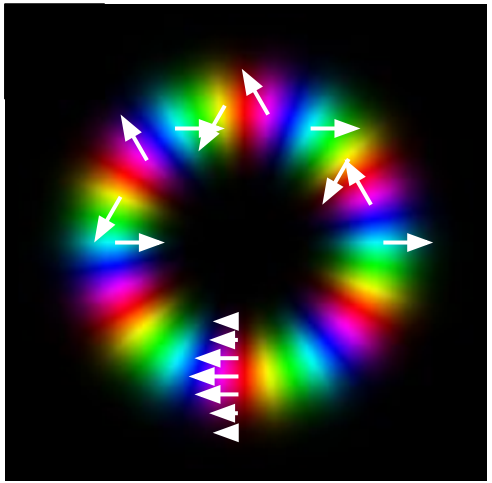
Step 1: Orientation field

$$\phi = \{[(\psi - \min(\psi)) * K][\psi - \min(\psi)]\} * G$$

$$K(\boldsymbol{k}) = \exp\left[-(|\boldsymbol{k}| - q)^2 / (2\sigma^2) + i\, m \arg(\boldsymbol{k})\right]$$



$K(\boldsymbol{k}), m = 6$



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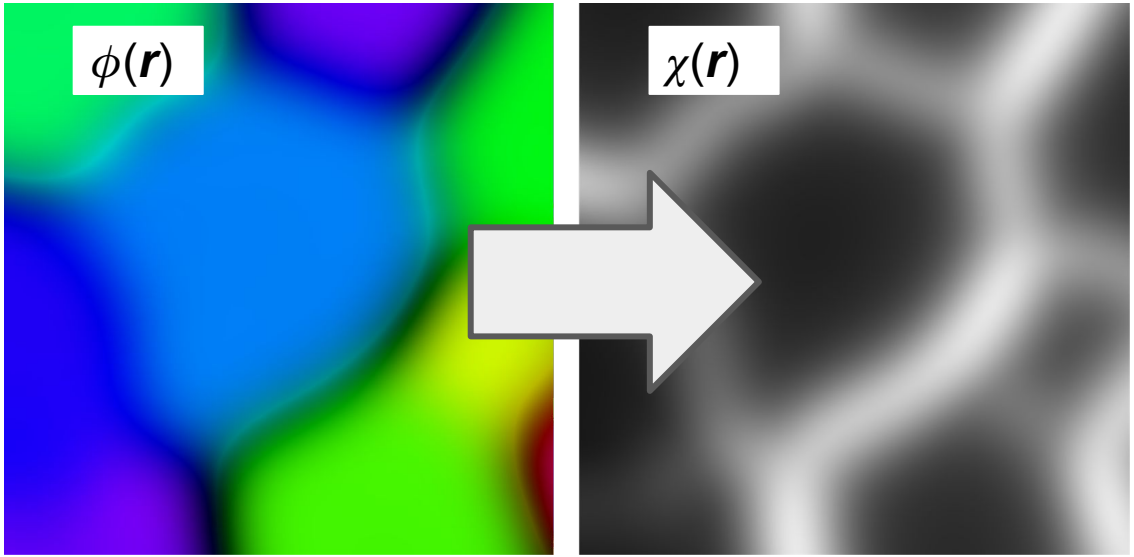
Grain extraction method

Step 2: Deformation field

$$\chi = \sum_{n=0}^{2^n a < \min(W,H)/2} \frac{|\nabla\phi|^p * \exp\left[-|\boldsymbol{r}|^2 / \left(2 \cdot 2^{2n} a^2\right)\right]}{\max\left\{|\nabla\phi|^p * \exp\left[-|\boldsymbol{r}|^2 / \left(2 \cdot 2^{2n} a^2\right)\right]\right\}}$$

$$|\nabla\phi| = \sqrt{\Re\left(\phi_x\right)^2 + \Im\left(\phi_x\right)^2 + \Re\left(\phi_y\right)^2 + \Im\left(\phi_y\right)^2}$$



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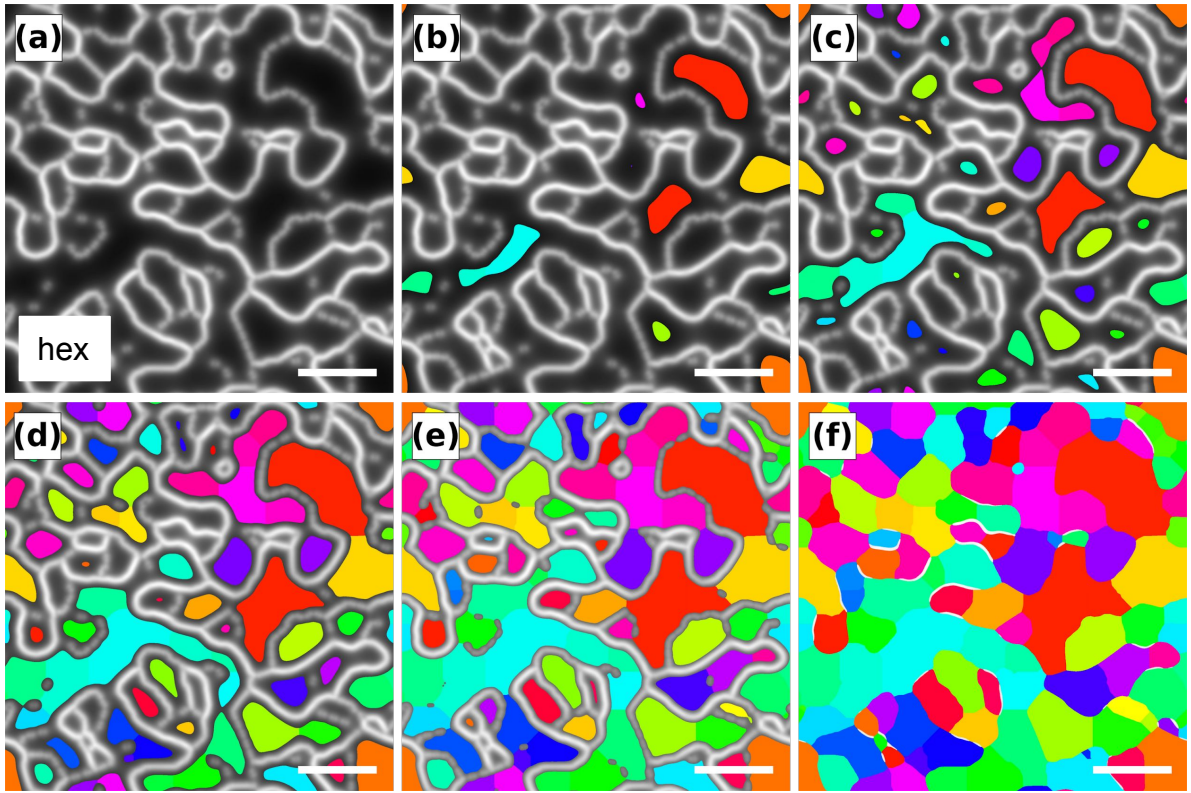
Grain extraction method

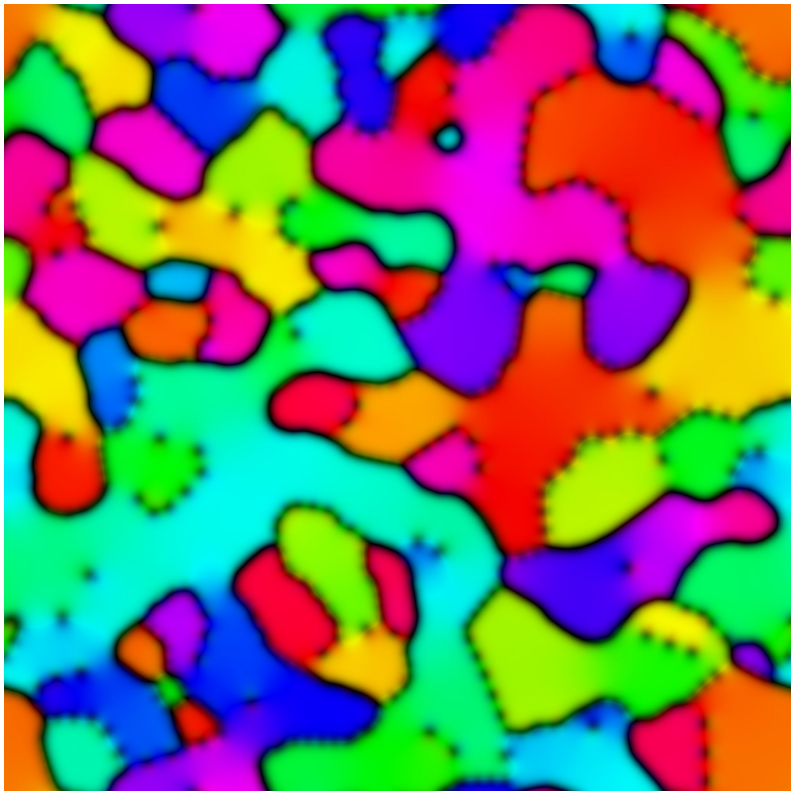
Step 3: Subdomain growth

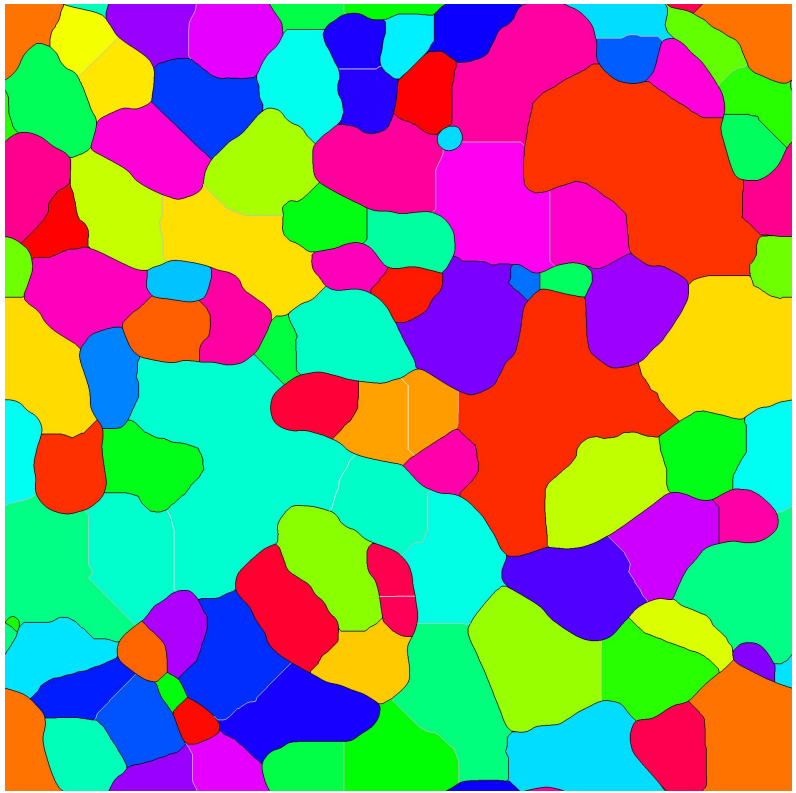


scale bar 40
lattice constants

Grain extraction method

Step 4: Subdomain merging





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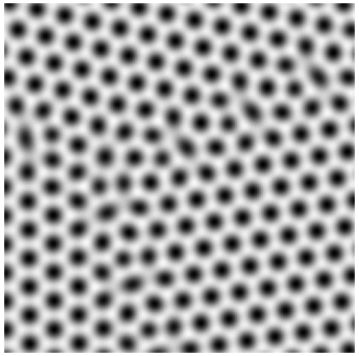
PFC model systems
Basics of PFC[a]

- PFC very well suited for generating realistic microstructures[b]
- Simple density functional approach to crystalline materials
- Main advantage access to long, diffusional time scales
- Can handle mesoscopic systems with atomic resolution
- Two main components
  - Smooth classical density field ψ
  - Governing free energy functional *F(ψ)*

$$F = \int d\boldsymbol{r} \left(\frac{\psi}{2} \left(R + \left(1 + \nabla^2 \right)^2 \right) \psi + \frac{\psi^4}{4} \right)$$



[a] *Elder et al., Phys. Rev. Lett.* ***88*** *(2002); Elder et al., Phys. Rev. E* ***70*** *(2004)*
[b] *Hirvonen et al., Phys. Rev. B* ***94*** *(2016); Hirvonen et al., Sci. Rep.* ***7*** *(2017); Fan et al., Nano Lett.* ***17*** *(2017); Azizi et al., Carbon* ***125*** *(2017)*

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PFC model systems
Two-mode PFC model[a, b]

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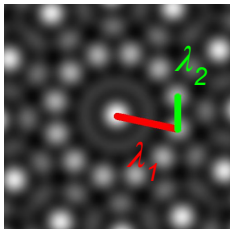
- Two competing length scales $\lambda_n \sim 1/q_n$
  - More lattices: square, hexagonal, 10-fold and 12-fold
- This and other PFC models used previously in studies related to quasicrystals
  - Growth modes[b]
  - Interfaces[c]
  - Monolayers on quasi-crystalline surfaces[d]
  - Three-dimensional quasicrystals[e]

$$F = \int d\boldsymbol{r} \left(\frac{\psi}{2} \left(R + \prod_{n=1}^{2} \left(q_n^2 + \nabla^2 \right)^2 \right) \psi + \frac{\psi^4}{4} \right)$$



[a] *Wu et al., Phys. Rev. E 81 (2010)*
[b] *Achim et al., Phys. Rev. Lett. 112 (2014)*
[c] *Schmiedeberg et al., Phys. Rev. E 96 (2017)*
[d] *Rottler et al., J. Phys. Condens. Matt. 24 (2012)*
[e] *Subramanian et al., Phys. Rev. Lett. 117 (2016)*

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Assessment of grain extraction method

Subdomain network

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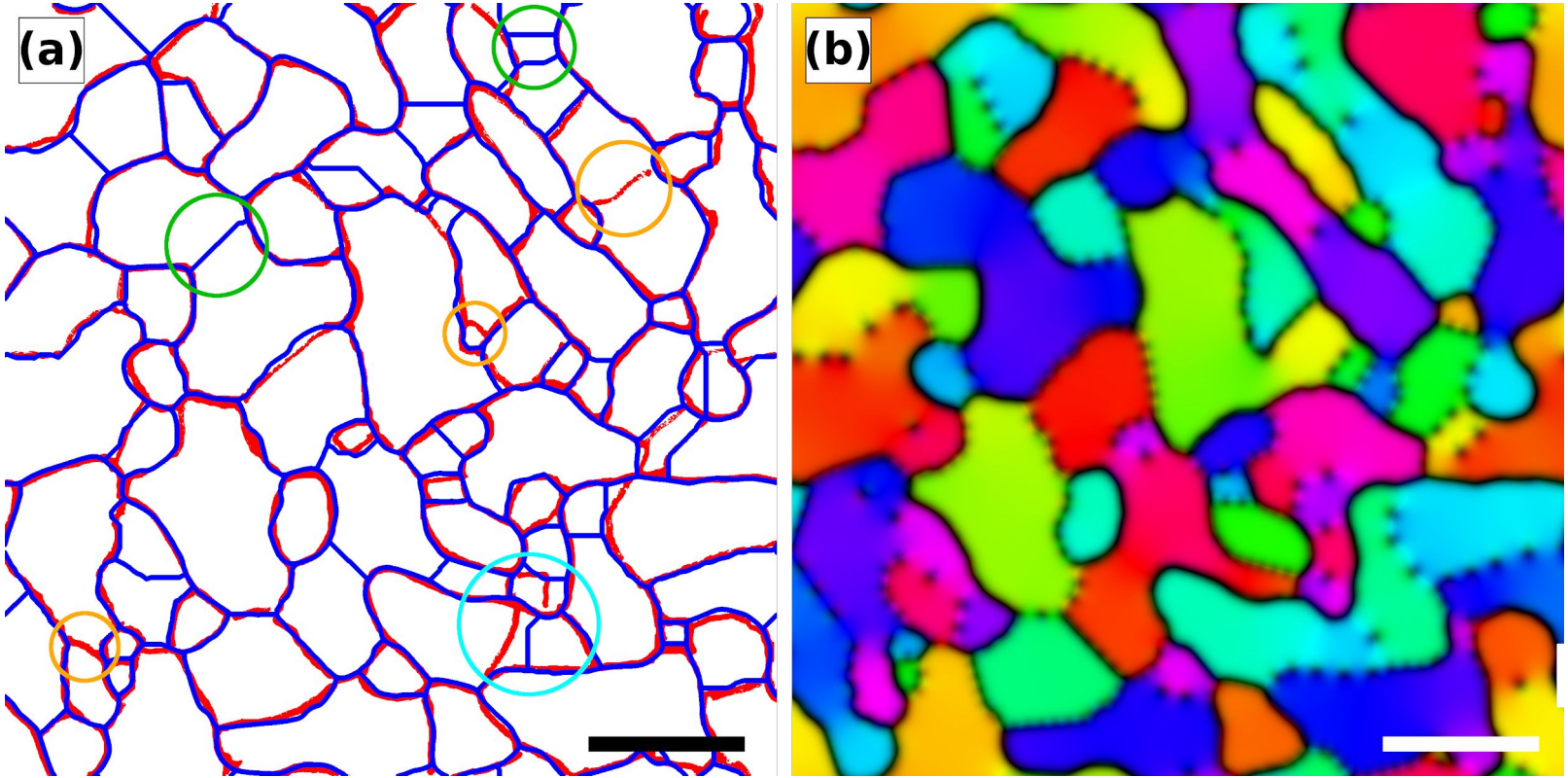

scale bar
40 lattice
constants

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Assessment of grain extraction method

Subdomain merging

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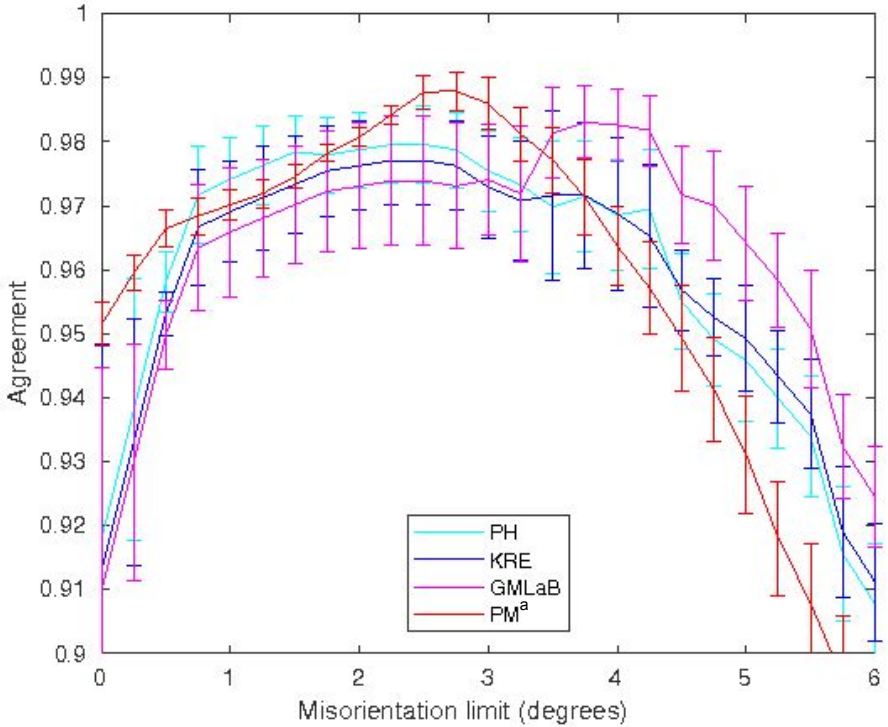

[a] *Boissonière et al., Model. Simul. Mater. Sci. Eng.* ***26*** *(2018))*

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Assessment of grain extraction method

Subdomain merging

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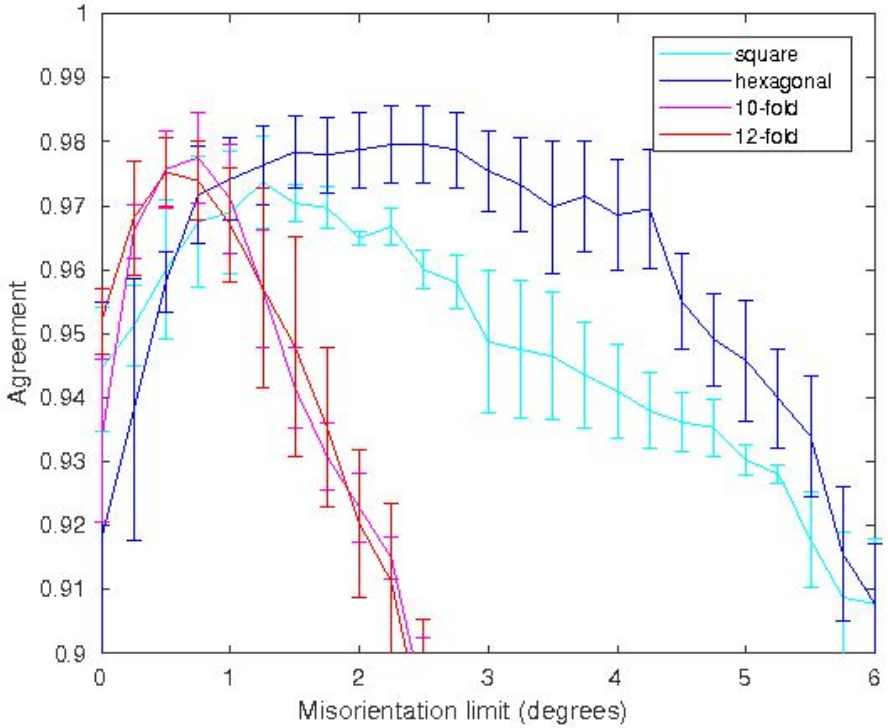

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Analysis of different microstructures

Evolution of average grain size

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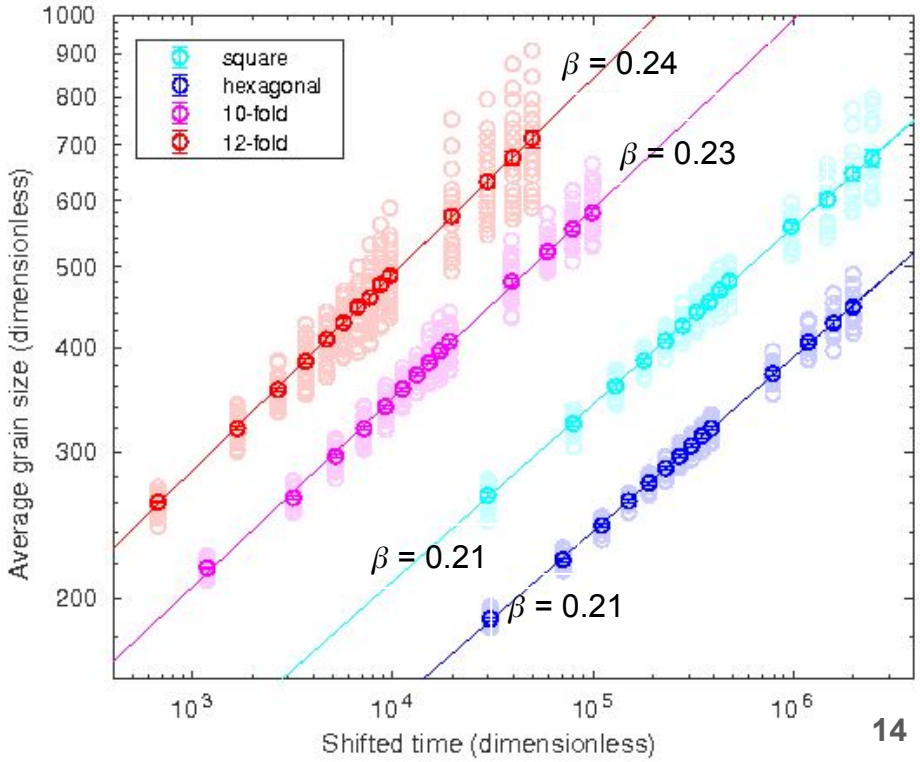
- Power-law growth expected[a, b, c]

$$\langle d(t) \rangle = \alpha \left(t + t_0 \right)^{\beta}$$

- All lattice types demonstrate perfect power-law growth
  - β = 0.21 - 0.24
- Hexagonal: good agreement with Backofen et al.[d]



[a] *Burke, Trans. Metall. Soc. AIME* ***180*** *(1949)*
[b] *Burke and Turnbull, Prog. Metal. Phys.* ***3*** *(1952)*
[c] *Krzanowski et al., Acta Metall.* ***34*** *(1986)*
[d] *Backofen et al., Acta Mater.* ***64*** *(2014)*

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Analysis of different microstructures

Normalized grain size distributions

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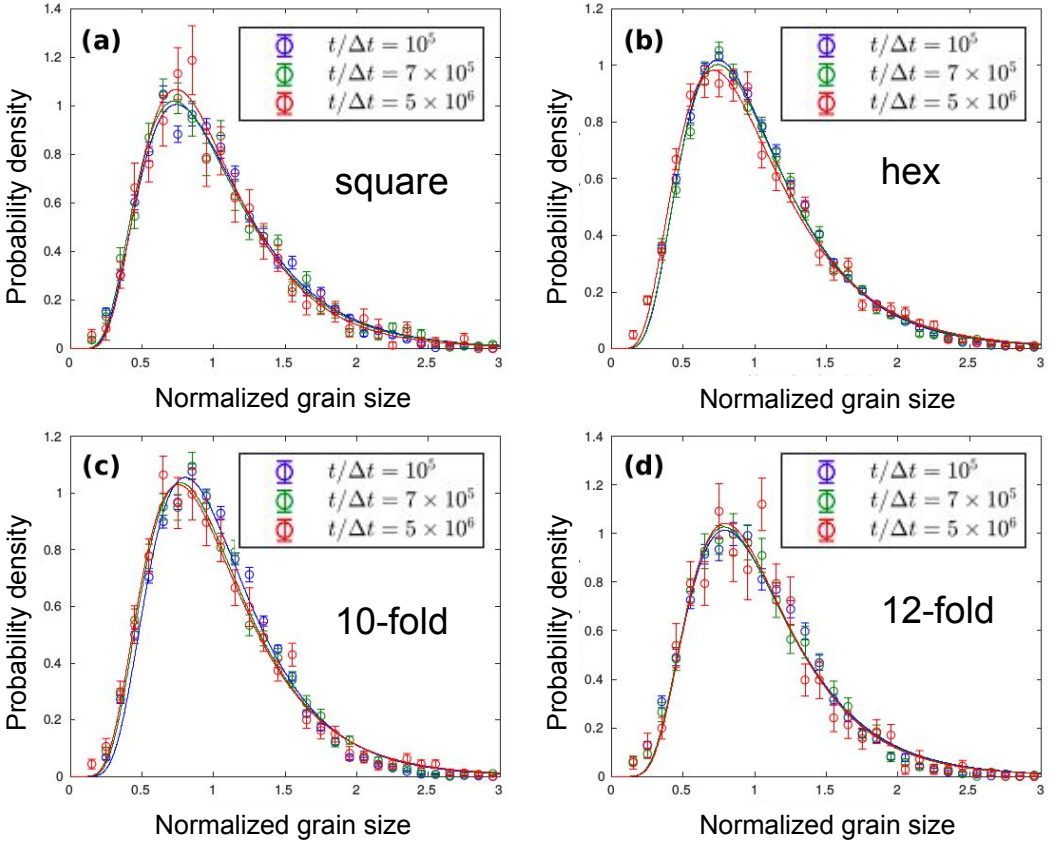
- Log-normal distributions both expected[a, b, c] and observed
- All lattice types demonstrate identical behavior



[a] *Backofen et al., Acta Mater.* ***64*** *(2014)*
[b] *La Boissonière et al., Model. Simul. Mater. Sci. Eng.* ***26*** *(2018)*
[c] *Barmak et al., Prog. Mater. Sci.* ***58*** *(2013)*

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Analysis of different microstructures

Grain size ratio distributions

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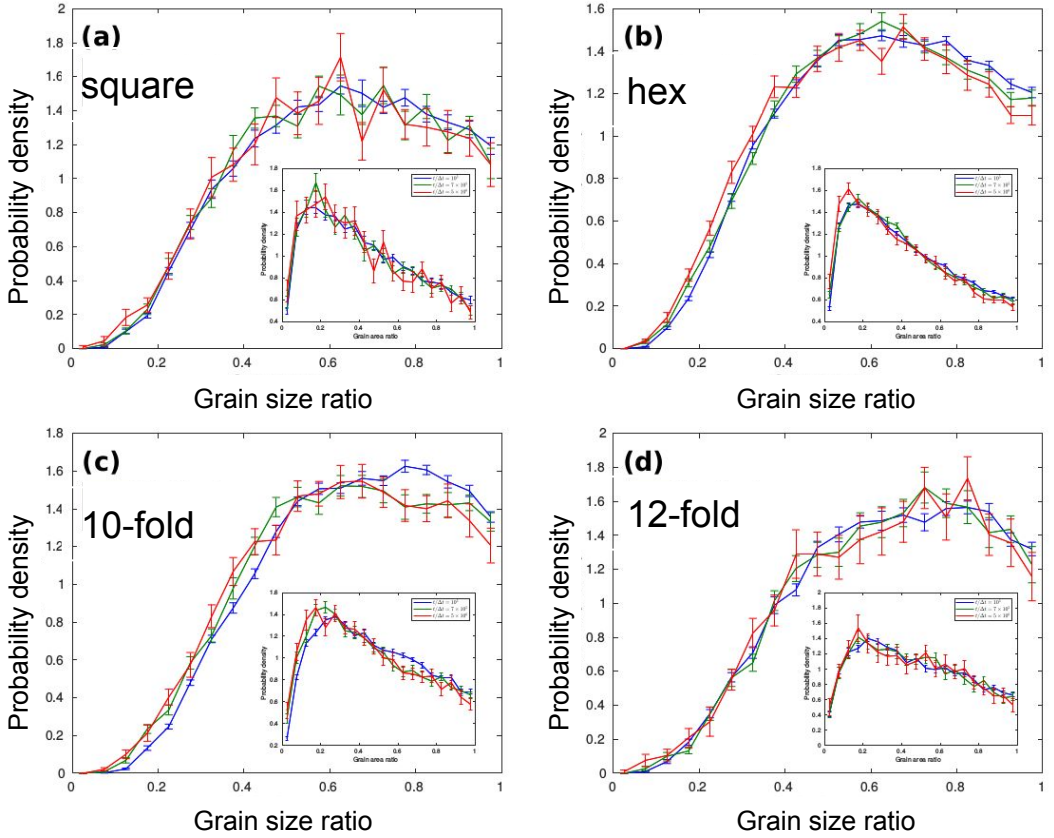
- All lattice types favor similar disparity in grain size between neighbors
  - $\langle\delta\rangle$ = 0.62, 0.61, 0.64, 0.64
- Hexagonal: grain area ratio very similar to La Boissonière et al.[a]



[a] *La Boissonière et al., Model. Simul. Mater. Sci. Eng.* ***26*** *(2018)*

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Analysis of different microstructures

Grain misorientation distributions

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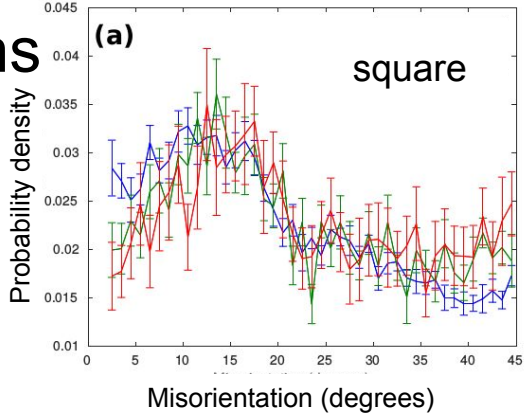
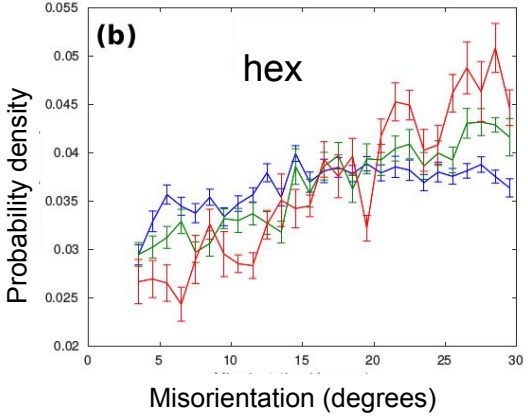
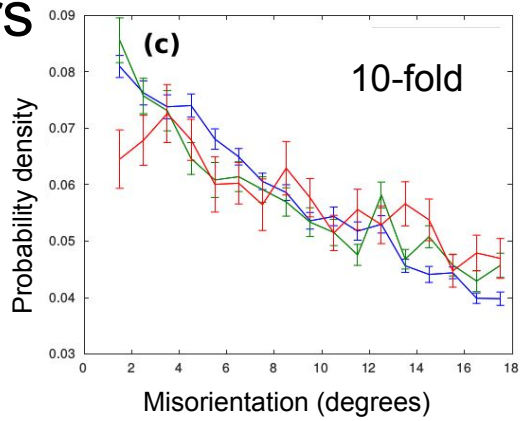
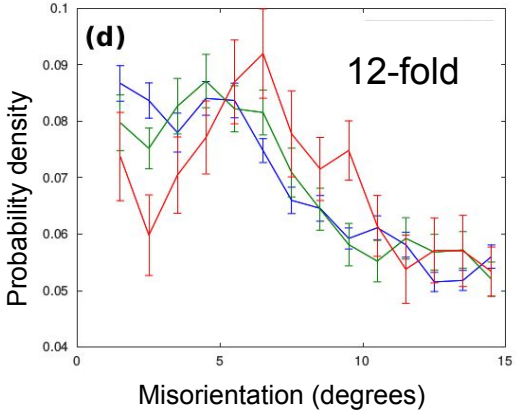
- Very different distributions for different lattice types!
- Hexagonal: favors large misorientations
  - Previous[a]: small!
  - Model and parameters
- Square: bump at ~15°
- 12-fold: bump at ~7°
- Grain boundary energy?









[a] *La Boissonière et al., Model. Simul. Mater. Sci. Eng.* ***26*** *(2018)*

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Conclusions

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- A new accurate method for extracting grains and analyzing microstructures in poly(quasi)crystals was introduced and assessed[a]
- Applied to study microstructures of different lattice types[a]
  - Many properties universal beyond lattice type
  - Lattice misorientations show unique behavior
- We expect our method can greatly facilitate the study of complex microstructures in quasicrystals

[a] *Hirvonen et al., Grain extraction and microstructural analysis method for two-dimensional poly and quasicrystalline solids, submitted to Phys. Rev. Materials (June 2018),* ***arXiv:1806.00700***

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Thanks!

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- Collaborators
  - Gabriel Martine La Boissonière (McGill University)
  - Zheyong Fan (Aalto University)
  - Cristian-Vasile Achim (University of Concepcíon)
  - Nikolas Provatas (McGill University)
  - Ken Elder (Oakland University)
  - Tapio Ala-Nissila (Aalto Univ., Loughborough Univ.)
- You
- P.S. In case you forgot, my info:
  - Petri Hirvonen, petri.hirvonen@aalto.fi, MSP, Aalto Univ.

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Obtaining the orientation field

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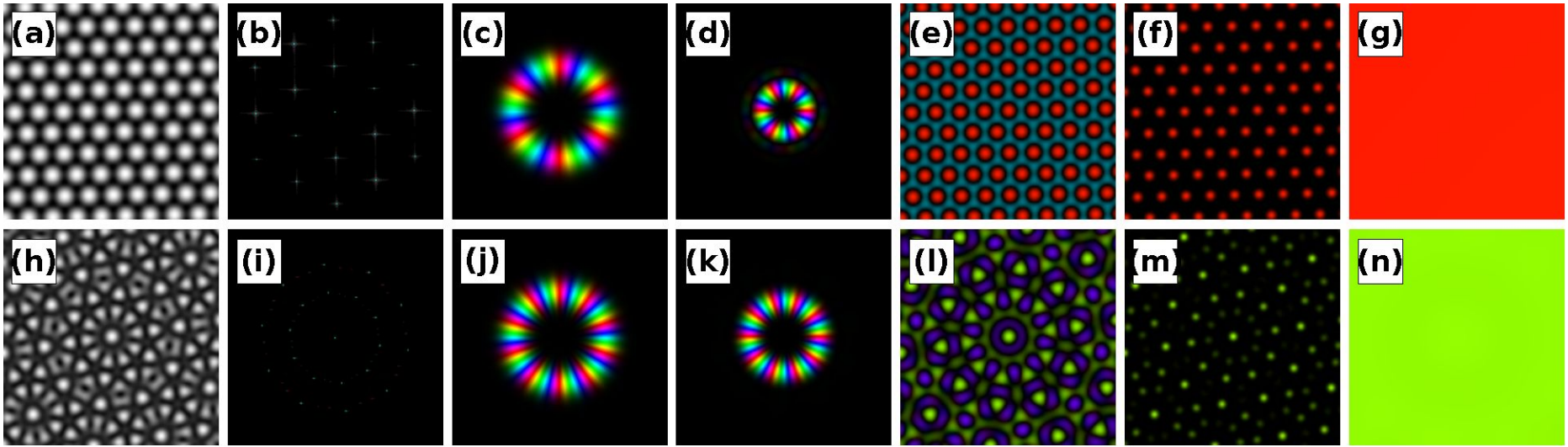

PFC model systems
Construction of model systems

- Properties
  - Periodic boundaries
  - Planar
  - Free-standing
- Random tiled initial state
  - For stability
- Diffusive PFC dynamics

$$\frac{\partial \psi}{\partial t} = \nabla^2 \frac{\delta F}{\delta \psi}$$

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Assessment of grain extraction method

Applicability to molecular dynamics data

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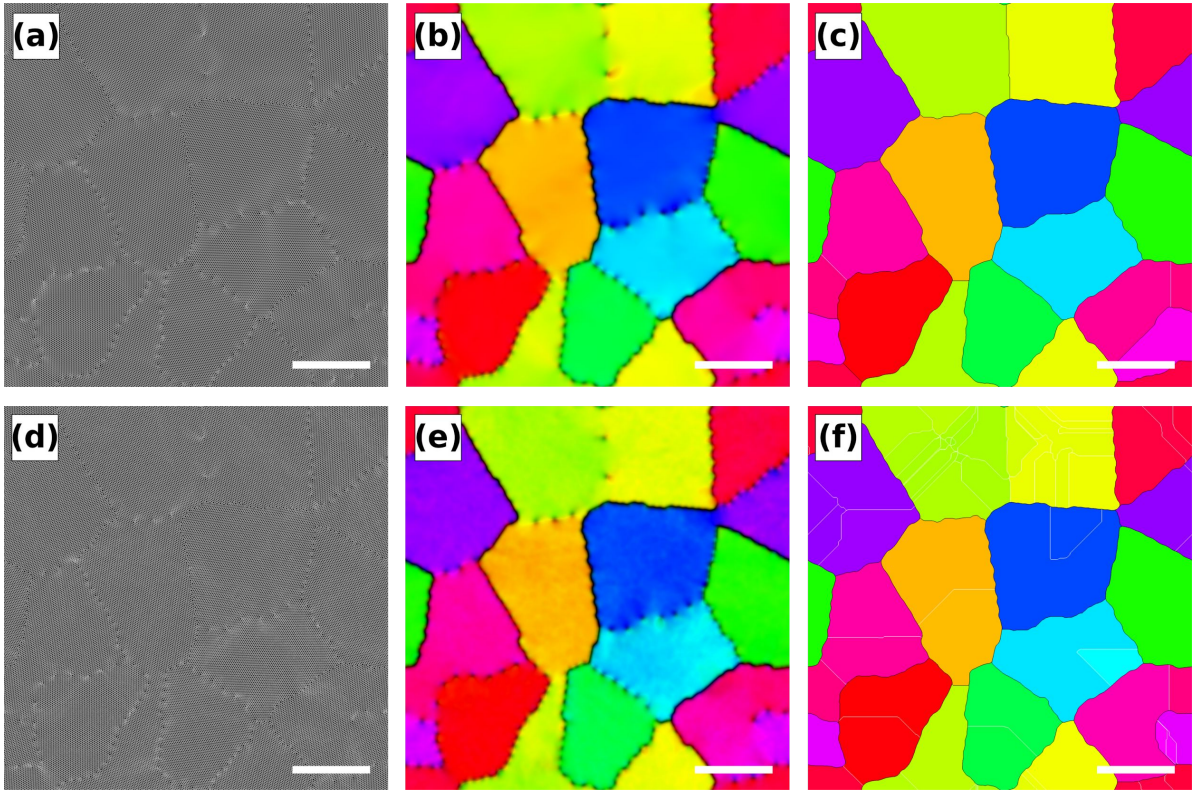

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Paper scraps

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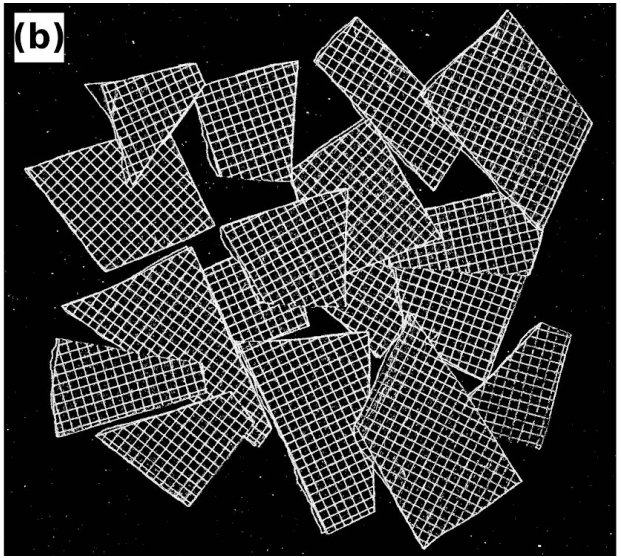

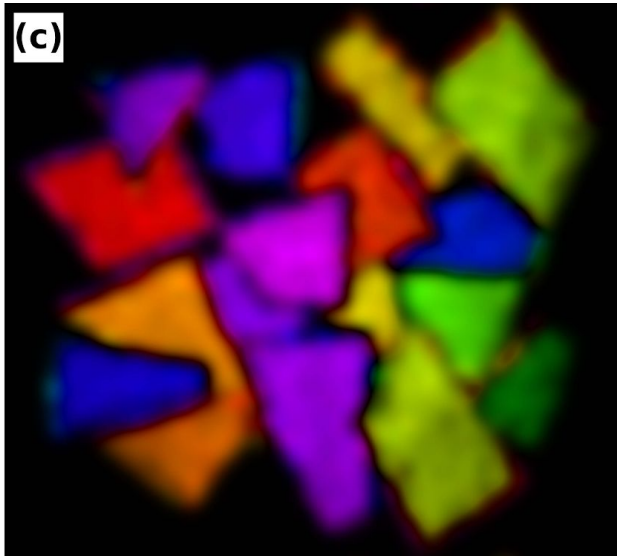

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Stripe systems

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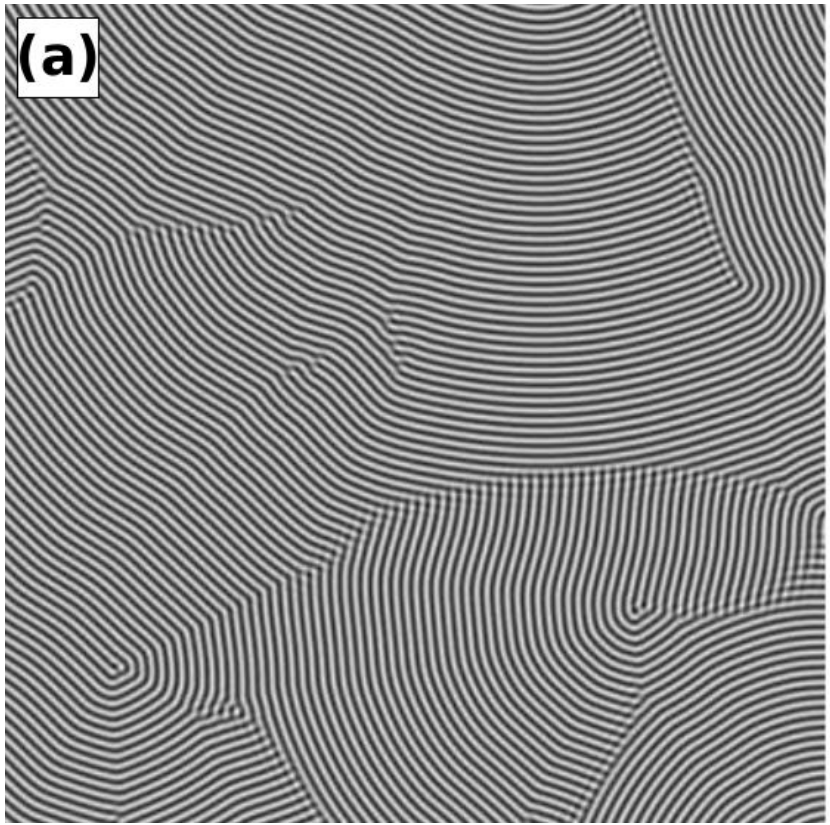

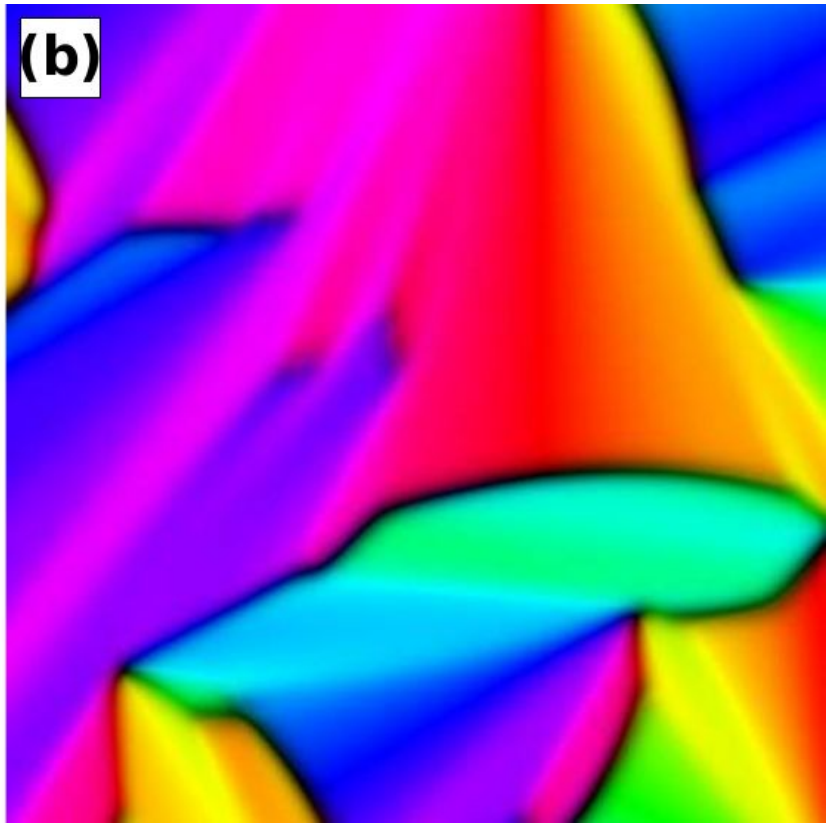

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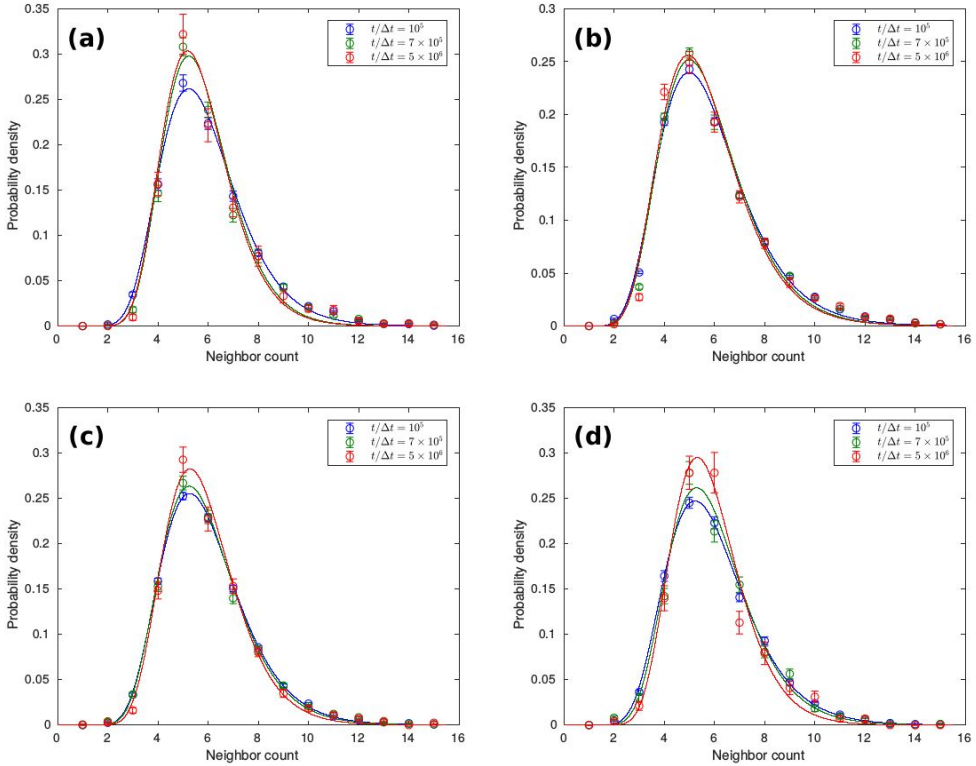
Further results
Grain neighbor count distributions



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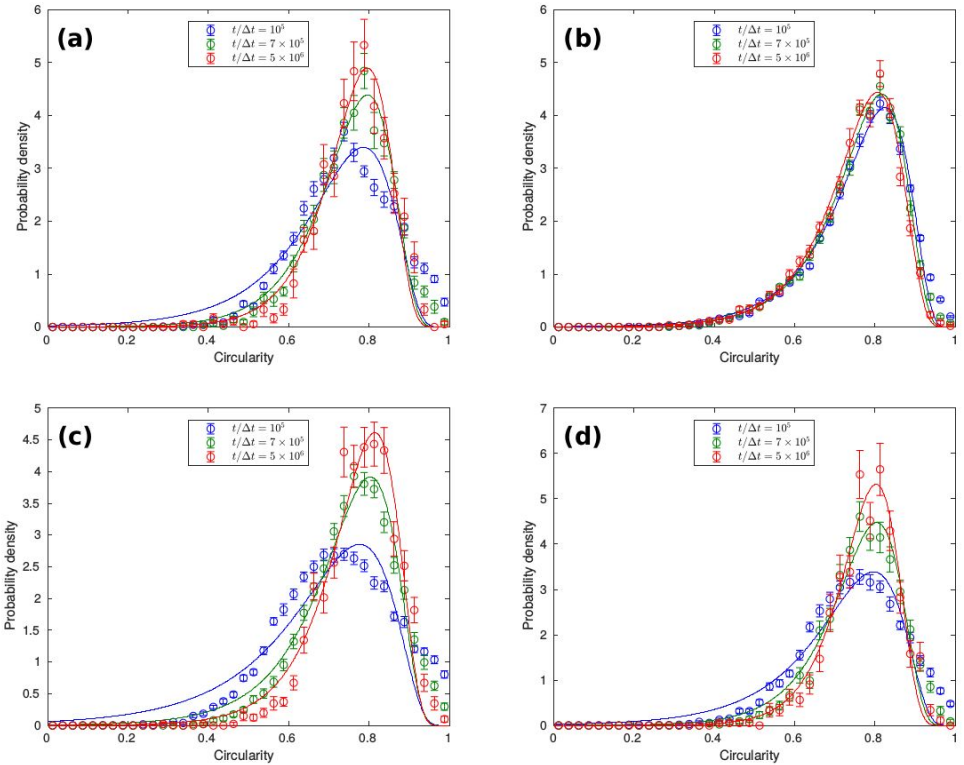
Further results
Grain circularity distributions



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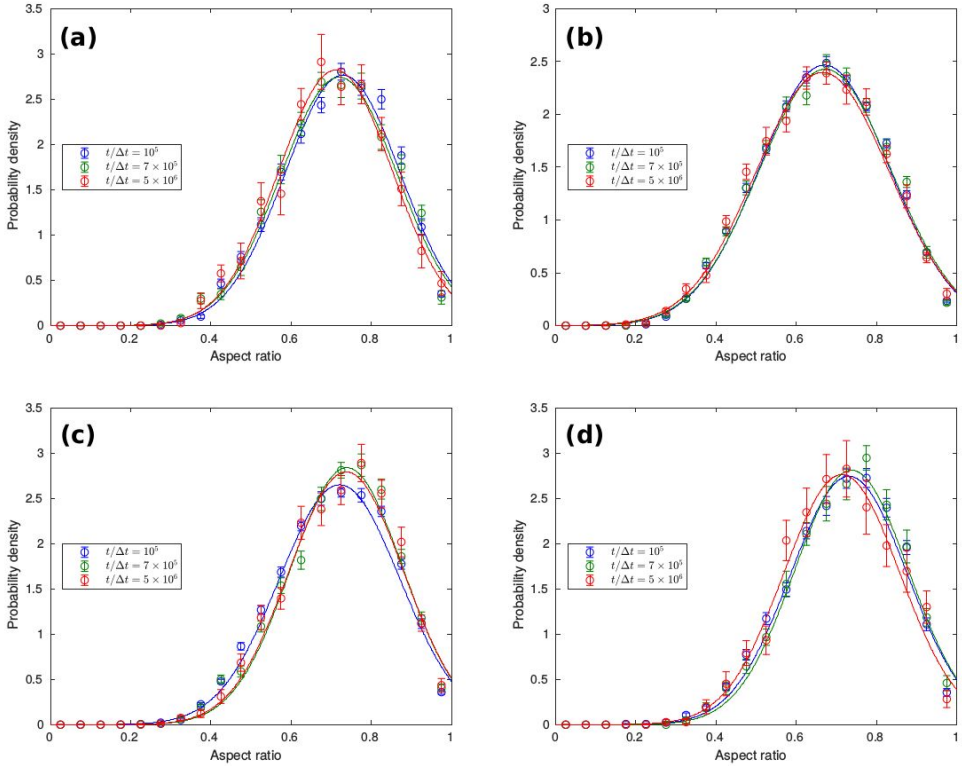
Further results
Grain aspect ratio distributions



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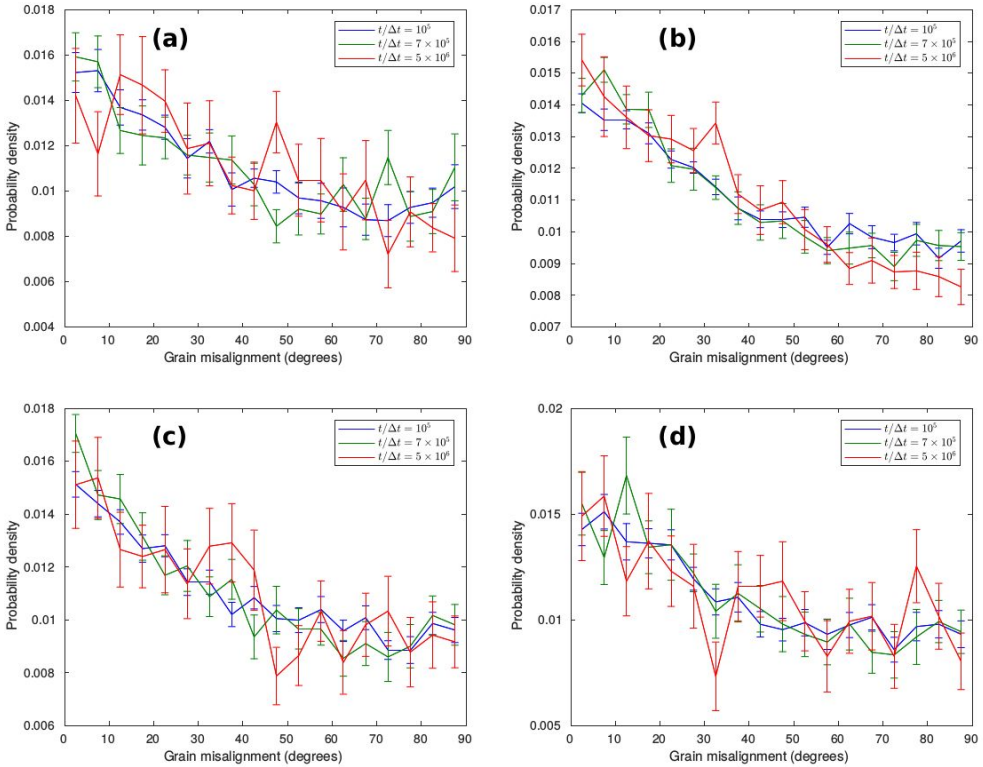
Further results
Grain misalignment distributions



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Computational performance

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- Benchmark
  - 8192 x 8192 system with 1084 grains
  - Quad-core (Intel Xeon E3-1230 v5) PC
- Execution times (a few minutes in total)
  - ϕ + χ: ~90 s (more CPU cores → faster)
  - Subdomain growth: ~90 s (smarter parallel algorithm → much faster)*
  - Initialization + reading data: ~40 s *
  - Principal component analysis: ~60 s (optional)
- Maximal memory usage: ~10 GB (smarter algorithm → less)

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GB energy calculations
Details

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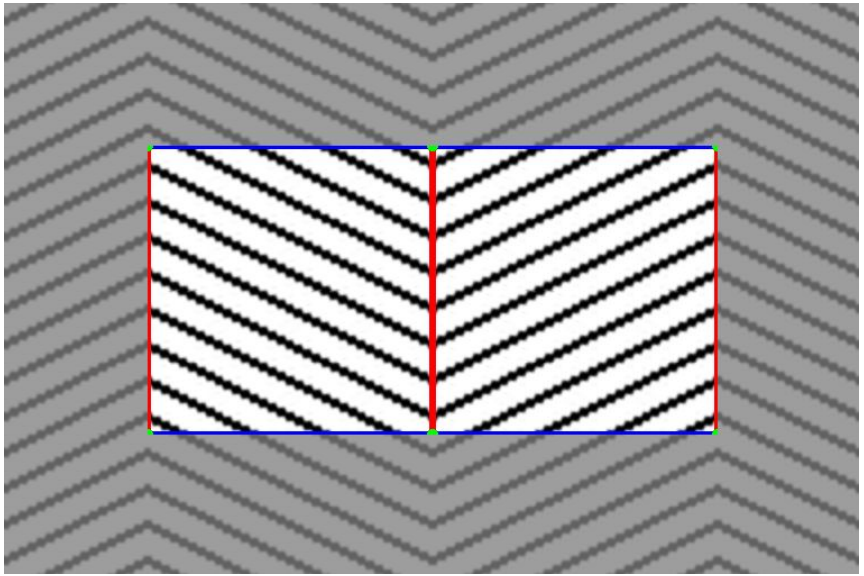
$$\gamma = \frac{L_\perp}{2}\left(f - f_{\mathrm{eq}}\right)$$



$$F = f_{\mathrm{eq}} S + 2\gamma L_{||} + \gamma^* L_\perp + 2\delta$$

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School of Science

GB energy calculations
Results

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