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Kinetic Monte Carlo Simulations of Structural Evolution of Additively Manufactured Materials

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Additive Manufacturing

Advantages

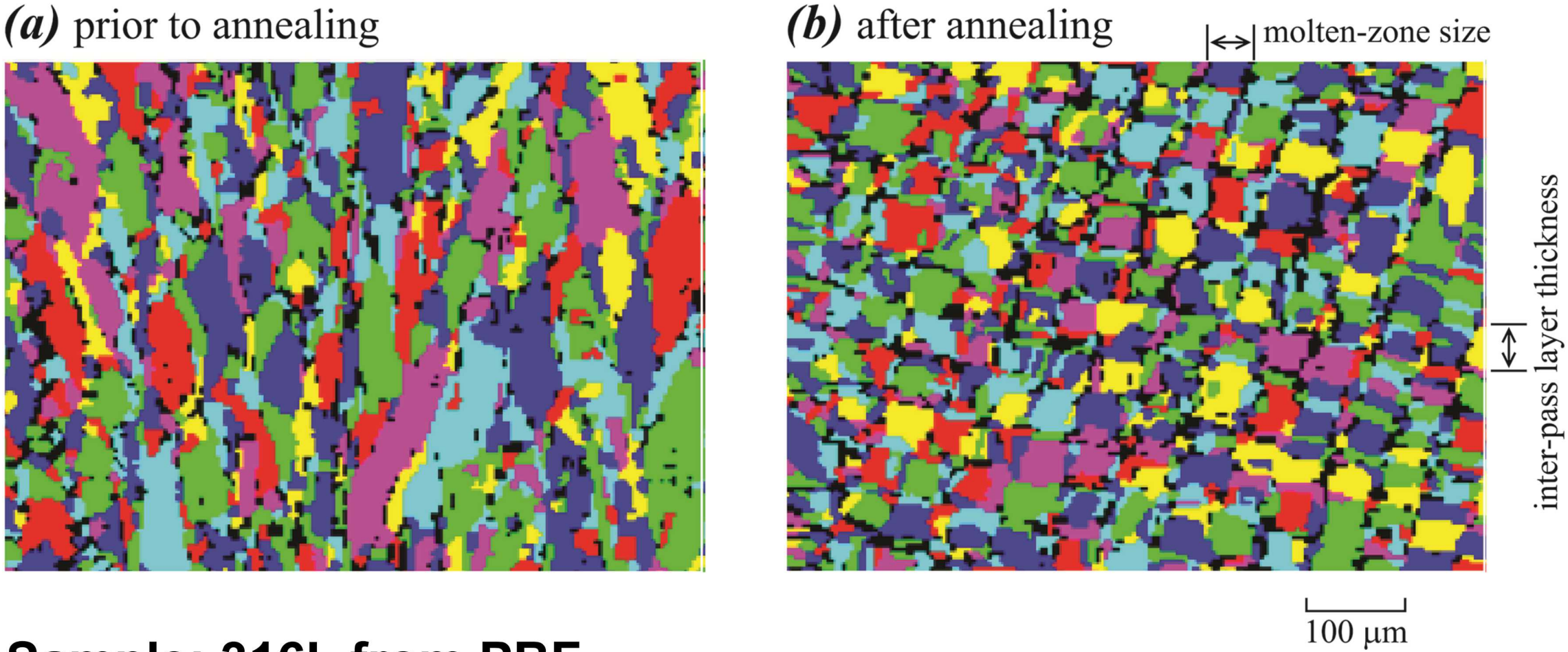
- Rapid prototyping
- Intelligent material design
- Low waste production
- Increased energy efficiency
- Reduced material cost

R&D Needs

- Insufficient data
- Large uncertainty margin
- Reduced stability
- Poor understanding

Predictive models are needed to promote understanding!

An Example of Microstructure Evolution

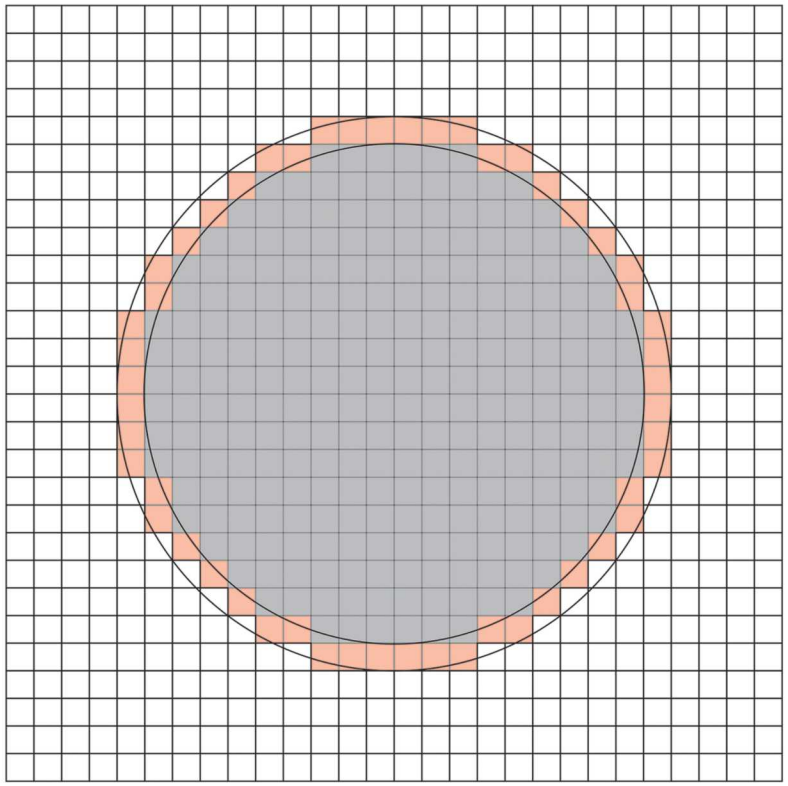


- Sample: 316L from PBF
- Annealing: from 25 to 1000°C at 6°C/min
- Analysis: EBSD

Objective: Predictive Simulations of Microstructural Evolution

- Develop a kinetic Monte Carlo (kMC) method incorporating:
  - Real time and length scales
  - Grain growth under driving energies
  - Recrystallization
- Identify model parameters
- Simulate and explain the observed microstructure evolution of the 316L PBF sample during annealing

Potts kMC Grain Growth Model



$$P = \begin{cases} exp\left(-\frac{\Delta E_\sigma}{kT}\right), & \Delta E_\sigma > 0 \\ 1, & \Delta E_\sigma \leq 0 \end{cases}$$

- A sample is divided into sites
- Each site has an integer number representing grain orientation
- Neighboring sites with different numbers bound a grain boundary
- Flipping number causes a grain boundary energy change ΔE_σ
- Continuously flipping the spin numbers at probability P

Our Modified Grain Growth Equations

- **Grain boundary mobility**

$$m = m_0 exp\left(-\frac{Q}{kT}\right)$$

- **Activation energy modified by grain boundary energy change**

$$\Delta Q_\sigma = c_\sigma \Delta E_\sigma$$

- **Grain orientation flipping rate (rather than probability)**

$$\Gamma_i = \begin{cases} \frac{\sigma m_0}{\Delta x^2} exp\left(-\frac{Q+\Delta Q_\sigma}{kT}\right), & Q + \Delta Q_\sigma > 0 \\ \frac{\sigma m_0}{\Delta x^2}, & Q + \Delta Q_\sigma \leq 0 \end{cases}$$

Further Addition of Driving Energies

- Each site is associated with an additional float number representing local stored energy
- Activation energy further modified if flipping a grain number also release local stored energy $c_e \Delta E_e$

$$\Delta Q_e = c_e \Delta E_e$$

- Grain orientation flipping rate is then

$$\Gamma_i = \begin{cases} \frac{\sigma m_0}{\Delta x^2} exp\left(-\frac{Q+\Delta Q_\sigma+\Delta Q_e}{kT}\right), & Q + \Delta Q_\sigma + \Delta Q_e > 0 \\ \frac{\sigma m_0}{\Delta x^2}, & Q + \Delta Q_\sigma + \Delta Q_e \leq 0 \end{cases}$$

kMC Simulation Steps

- Calculate flipping frequencies Γ_i^j for all sites i and all neighbors j
- Align Γ_i^j in a one-dimensional chain from 0 to $\Sigma_{i,j}\Gamma_i^j$. Generate a random number between 0 to $\Sigma_{i,j}\Gamma_i^j$. This random number points to a specific Γ_i^j event. Execute this event
- March the time forward by dt = $-\ln(\mathbb{R})/\Sigma_{i,j}\Gamma_i^j$ [1], where $\mathbb{R}$ is a random number between 0 and 1
- Repeat the process until total simulated time is consumed

1. A. B. Bortz, M. H. Kalos, and J. L. Lebowitz, A new algorithm for Monte Carlo simulation of Ising spin systems. J. Comput. Phys. 17, 10-18 (1975).

Recrystallization Model

- Nucleation event: assigning a new spin number and resetting stored energy to zero
- Nucleation rate [1]

$$\Gamma_i^n = \dot{n}_0 exp\left(-\frac{\Delta G^*}{kT}\right)$$

- Gibbs free energy of activation [1]

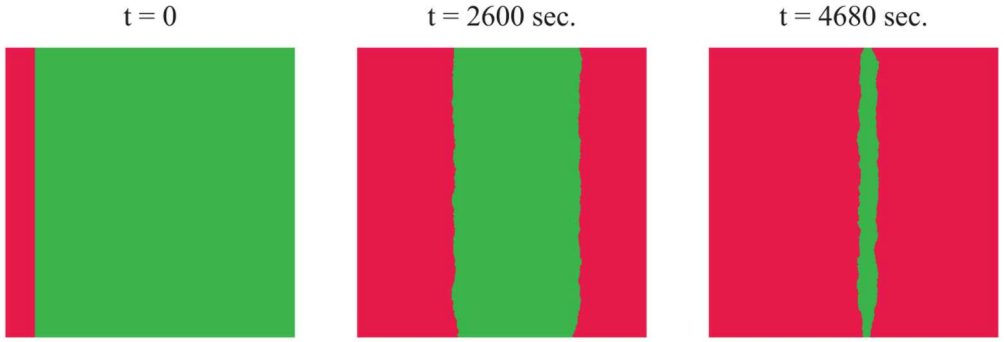
$$\Delta G^* = \frac{16\pi\sigma_n^3}{3e_i^2}$$

- The same kMC steps as described above is used except that $\Sigma_{i,j}\Gamma_i^j$ is replaced by $\Sigma_{i,j}\Gamma_i^j + \Sigma_{i,ei\neq 0}\Gamma_i^n$

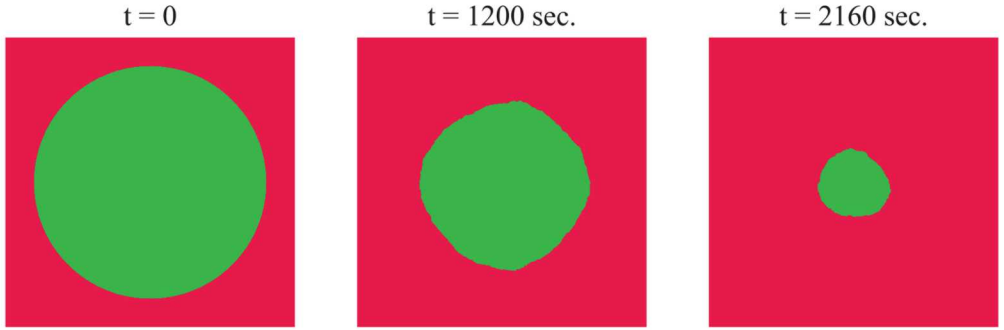
1. R. P. Sear, Nucleation: Theory and applications to protein solution and colloidal suspensions. J. Phys.: Condens. Matter, 19, 033101-28 (2007).

Validation Tests

(a) planar green domain at T = 550 K and e_i = 0.01 eV/Å^3

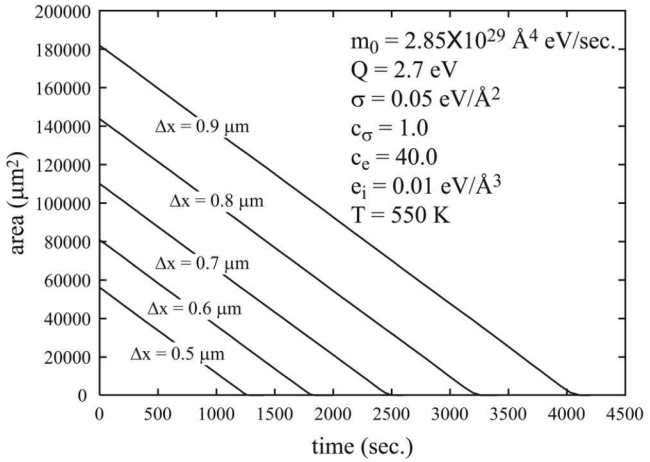


(b) circular green domain at T = 700 K and e_i = 0.00 eV/Å^3

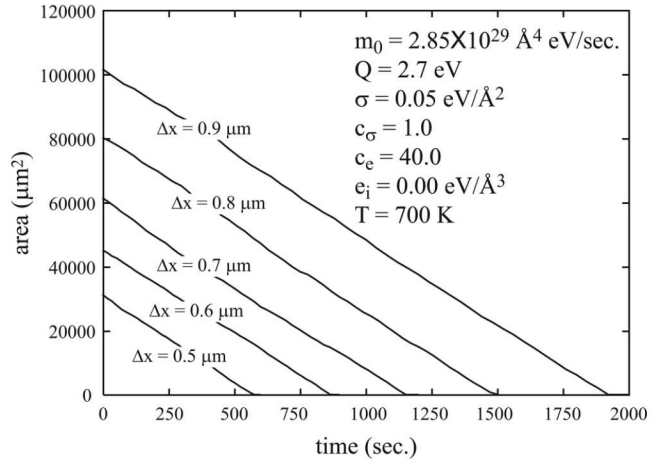


m_0 = 2.85X10^{29} Å^4 eV/sec., Q = 2.7 eV, σ = 0.05 eV/Å^2, c_σ = 1.0, c_e = 40.0 100 μm

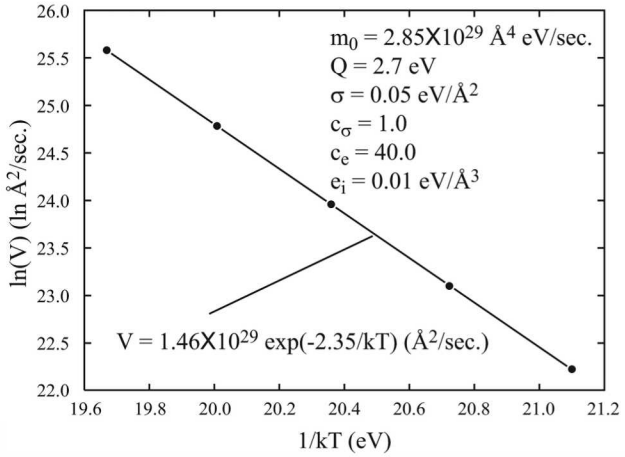
(a) planar case



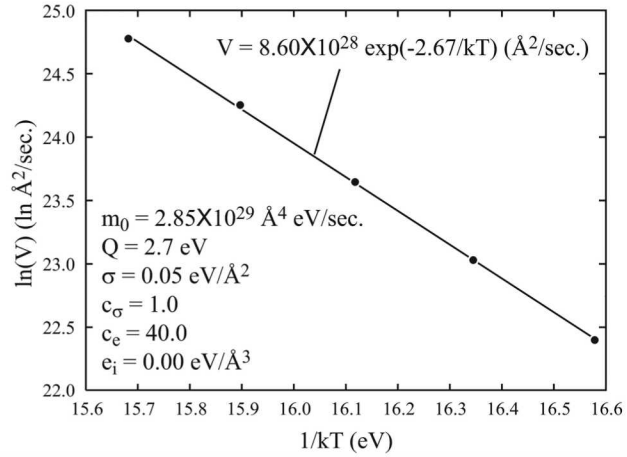
(b) circular case



(a) planar case



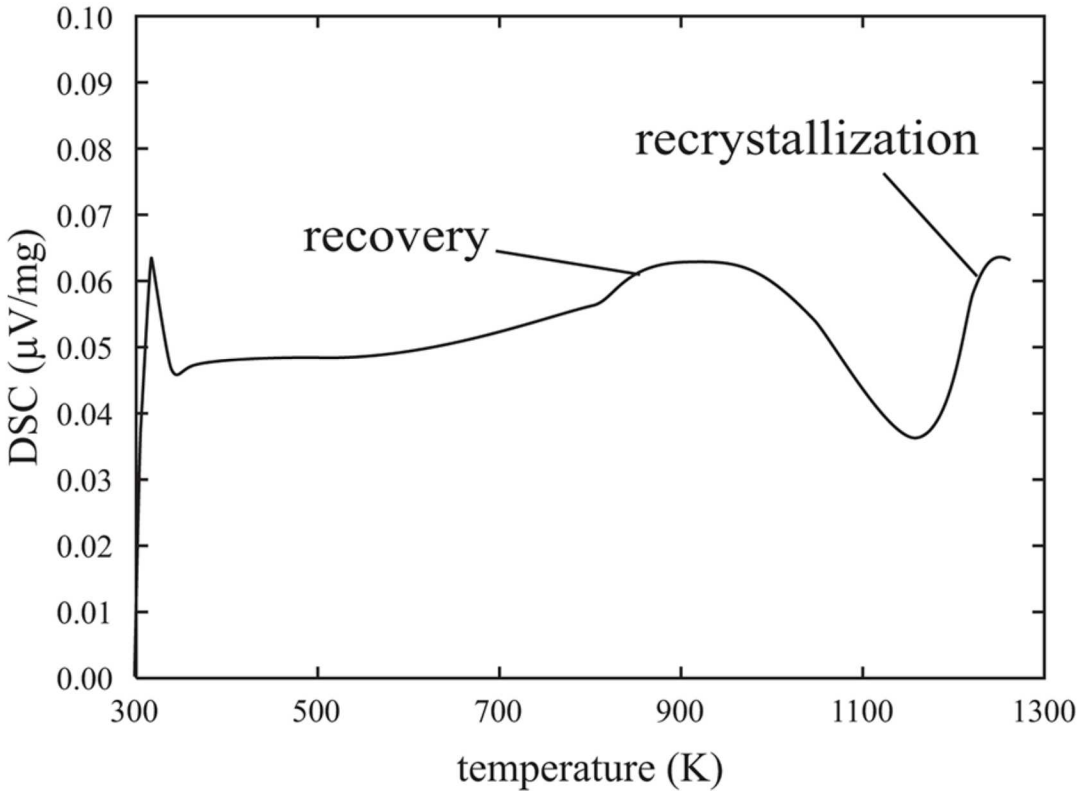
(b) circular case



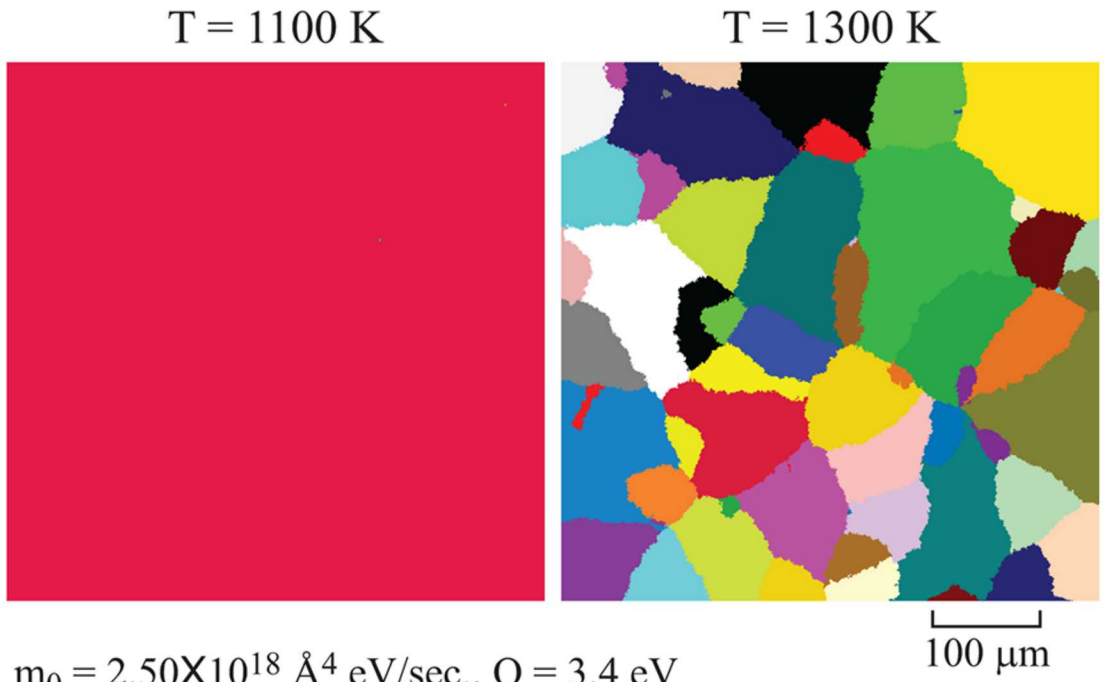
kMC simulations produced the expected results for a variety of test conditions.

Choices of Parameters

(a) DSC experimental results



(b) kMC from 300 K to 1300 K at 6 K/min.



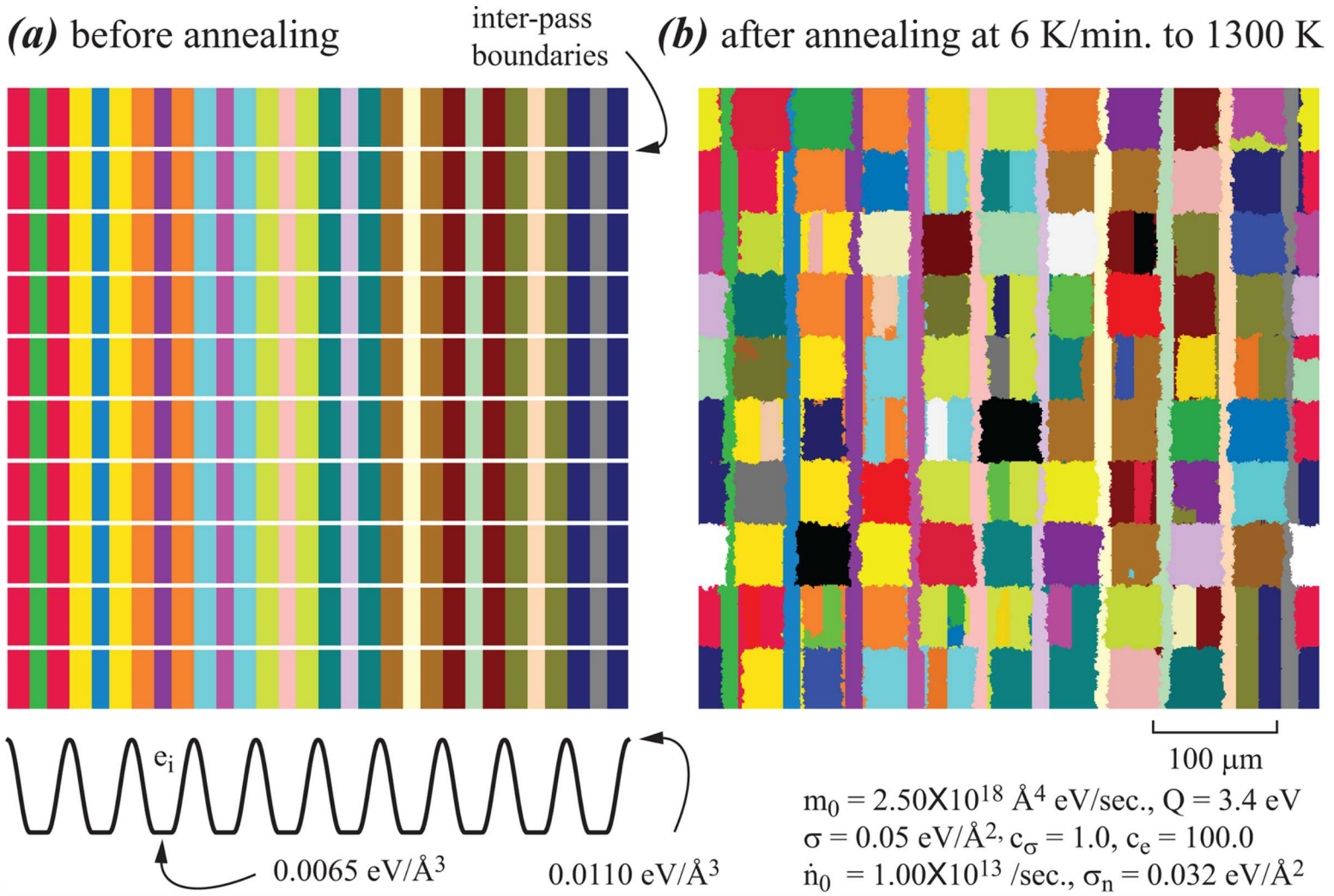
$m_0 = 2.50X10^{18}$ Å^4 eV/sec., Q = 3.4 eV

$\sigma = 0.05$ eV/Å^2, $c_\sigma = 1.0$, $c_e = 100.0$, $\dot{n}_0 = 1.00X10^{13}$ /sec.

$\sigma_n = 0.032$ eV/Å^2, $e_i = 0.011$ eV/Å^3

kMC simulation of a 316L sample annealed from 300 K to 1300 K at 6 K/min.

Predicted Microstructure Evolution



- The PBF produced 316L has stored energy periodically
- Model parameters are chosen to give phenomena seen from the DSC experiments
- Simulations predict the formation of cubic grain

Summaries

- A new kMC method with real time and length scales has been developed
- This kMC method incorporates grain growth, grain growth under a distribution of stored energy, and recrystallization
- The kMC parameters can be determined from DSC experiments during annealing from 300 to 1300 K
- Our kMC simulations indicate that periodically stored energy in a PBF manufactured 316L sample can cause the formation of cubic grains during annealing