

# Fundamentals of Crystal Growth



## Thermodynamics

- crystal potentials
- phase equilibrium
- phase relations
- surface/interface effects
- driving force of crystallization
- phase transition/nucleation

## Kinetics

- atomistic models
- interface description
- growth modes
- surface diffusion
- molecular-dynamics (MD) simulation
- in situ interface observation



## Transport

- heat (diffusion, convection, radiation)
- mass (diffusion, convection)





# Thermodynamics

- 1. Introduction**
- 2. Potential of Gibbs**
  - 2.1. The importance for crystal growth
  - 2.2. The point defect equilibrium
  - 2.3. The phase transition
- 3. Phase equilibrium**
  - 3.1. Two phases, one component
  - 3.2. Two phases, two components
  - 3.3. Phase diagrams
  - 3.4. Surfaces and interfacial effects
- 4. Deviation from equilibrium**
  - 4.1. Driving force of crystallization
  - 4.2. Nucleation (homo- and heterogeneous)
  - 4.3. Irreversible TD at crystal growth

# Kinetics



- 1. Introduction**
- 2. Atomistic models**
  - 2.1. Kossel-Stranski model
  - 2.2. PBC vectors
  - 2.3. Growth rate
  - 2.4. Surface diffusion
  - 2.5. Thermal roughening. Jackson model
  - 2.6. Kinetic roughening
- 3. Growth modes**
  - 3.1. Atomically rough interface
  - 3.2. Perfect singular face
  - 3.3. Vicinal face
  - 3.4. Face with screw dislocations
  - 3.5. Bunching effects
  - 3.6. Impurities
- 4. Molecular-dynamics (MD) simulation**

# Transport processes



- 1. Introduction**
- 2. Transport of heat**
  - 2.1. Conductivity
  - 2.2. Heat-balanced crystallization velocity
  - 2.3. Radiation
  - 2.4. Global numeric simulation
  - 2.5. Convection
- 3. Transport of mass**
  - 3.1. Diffusion
  - 3.2. Convection
  - 3.3. Macrosegregation
  - 3.4. Oscillation and microsegregation
  - 3.5. Counteractions and artificial mixing
- 4. Summary and Conclusions of the Lecture**