Crystal Shape Evolution in Detached Bridgman Growth

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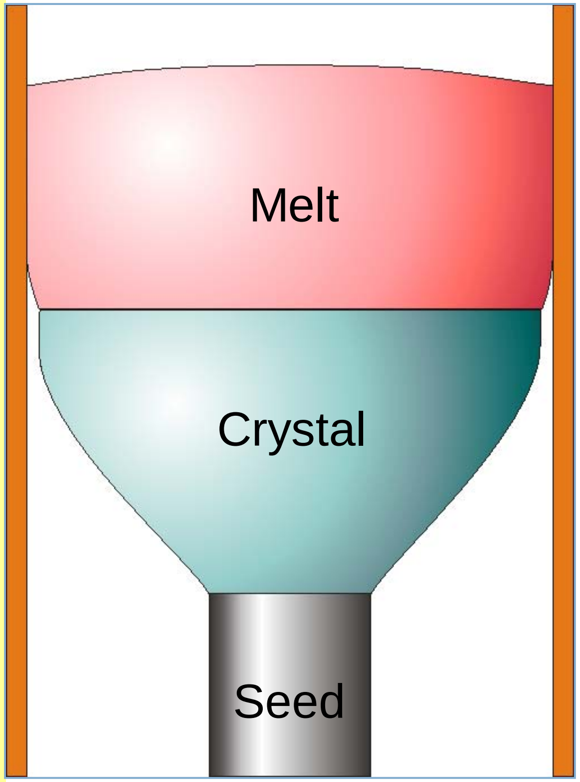
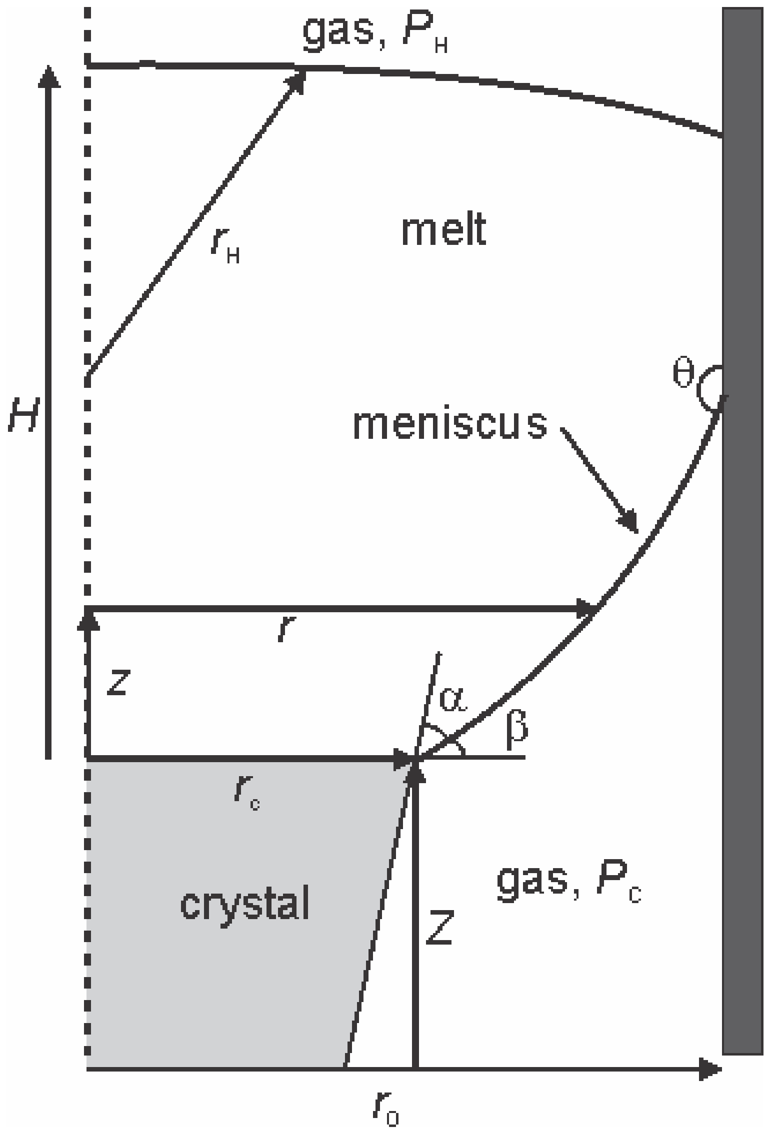
Research Motivation

- What are the conditions for detachment in microgravity and how do they depend on the governing parameters?
  - Growth angle
  - Contact angle
  - Pressure differential
  - Bond number (ratio of gravity to capillarity)
- Which detached growth solutions are dynamically stable?
- How does an initial crystal radius evolve to one of the following states?
  - Stable detached gap
  - Attachment to the crucible wall
  - Meniscus collapse
- What are the effects of angular dependence on the crystal shape (faceting effects)?



Schematic Diagram of Detached Solidification

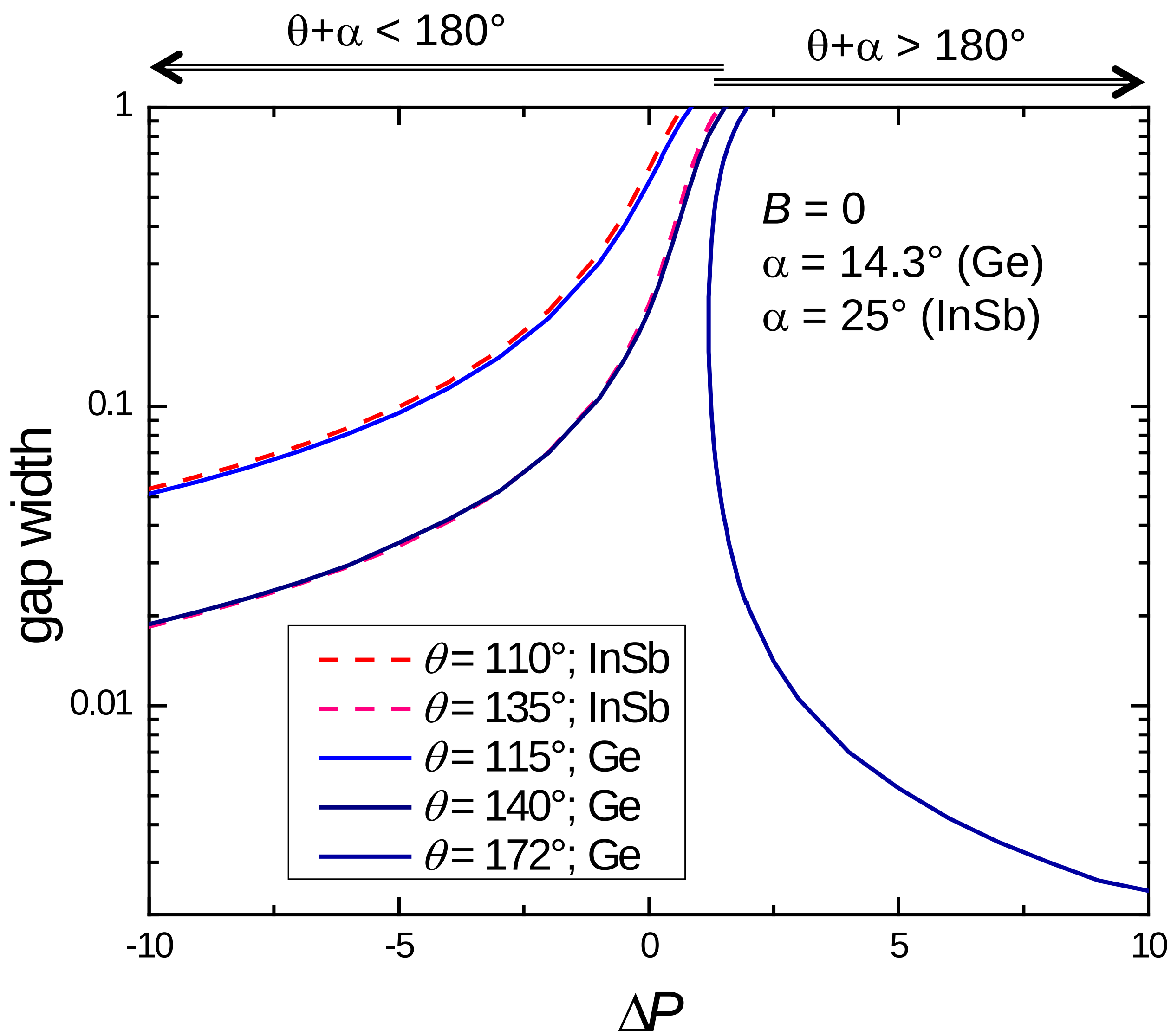


α: growth angle
θ: contact or wetting angle
$\Delta P = P_H - P_C$: Dimensionless pressure differential across the meniscus
$z(r)$: meniscus shape
$Z(r)$: crystal shape

Gap Width vs. Pressure Differential (Microgravity)

Equilibrium solutions

$$\frac{dr}{dZ} = 0$$

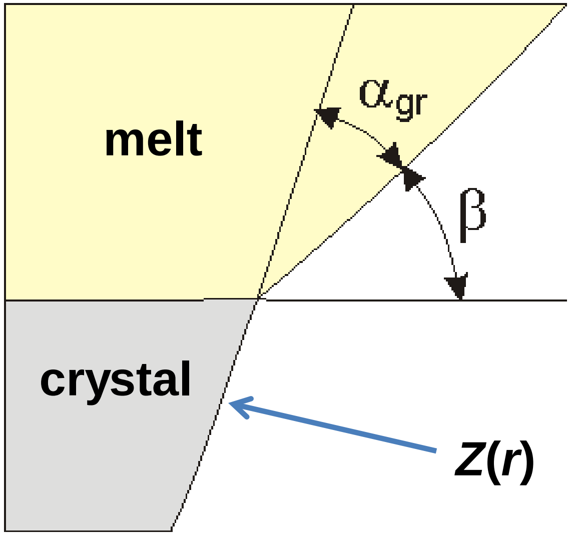


Equations in Zero Gravity

$$\frac{\partial z}{\partial r} = \pm \frac{\Delta P(r^2 - 1) - 2\cos\theta}{\sqrt{4r^2 - (\Delta P(r^2 - 1) - 2\cos\theta)^2}}$$

Meniscus shape equation, *z*(*r*): 2 possible solutions for *g* = 0, *B* = 0

$$\frac{dZ}{dr} = \tan(\alpha + \beta)$$



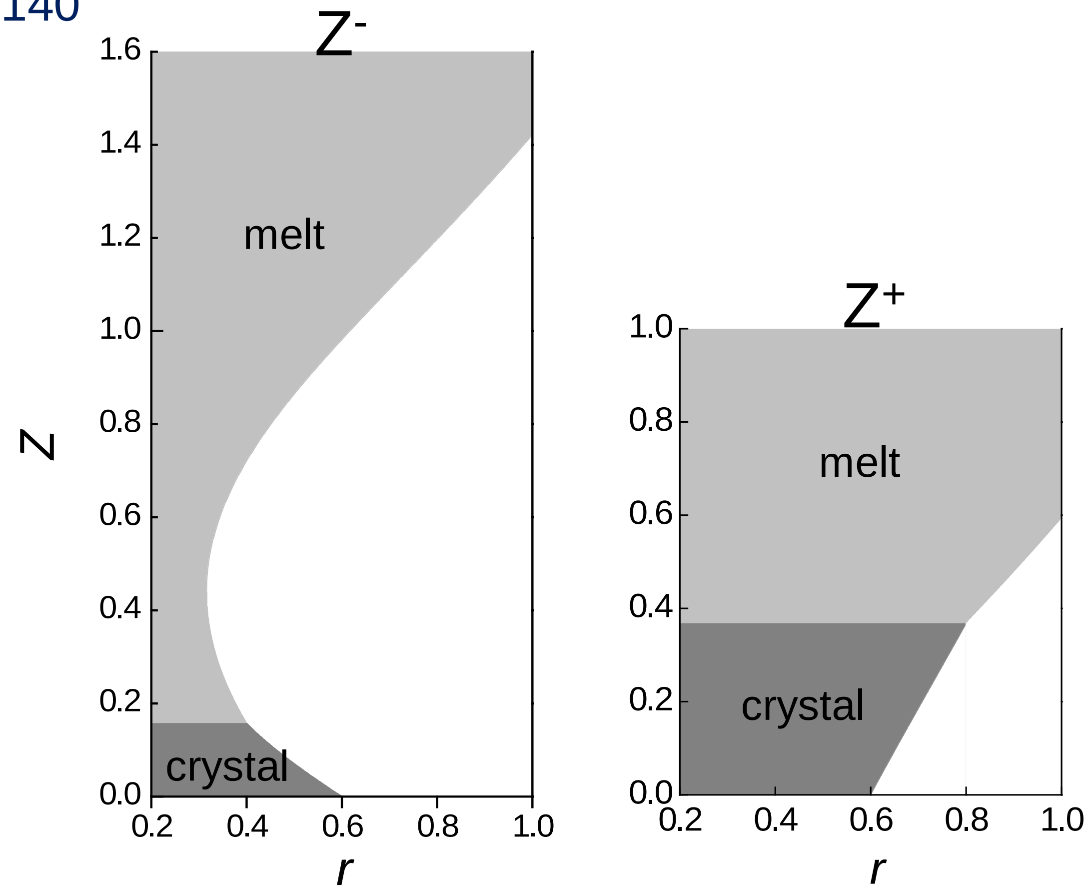
Crystal shape equation, *Z*(*r*): 2 possible solutions in zero gravity

$$\frac{dZ^{\pm}}{dr} = \frac{\sqrt{4r^2 - y^2}\,\tan\alpha \pm y}{\sqrt{4r^2 - y^2} \mp y\tan\alpha}, \qquad y = \Delta P(r^2 - 1) - 2\cos\theta$$

Two Solutions: Crystal Radius can Increase or Decrease

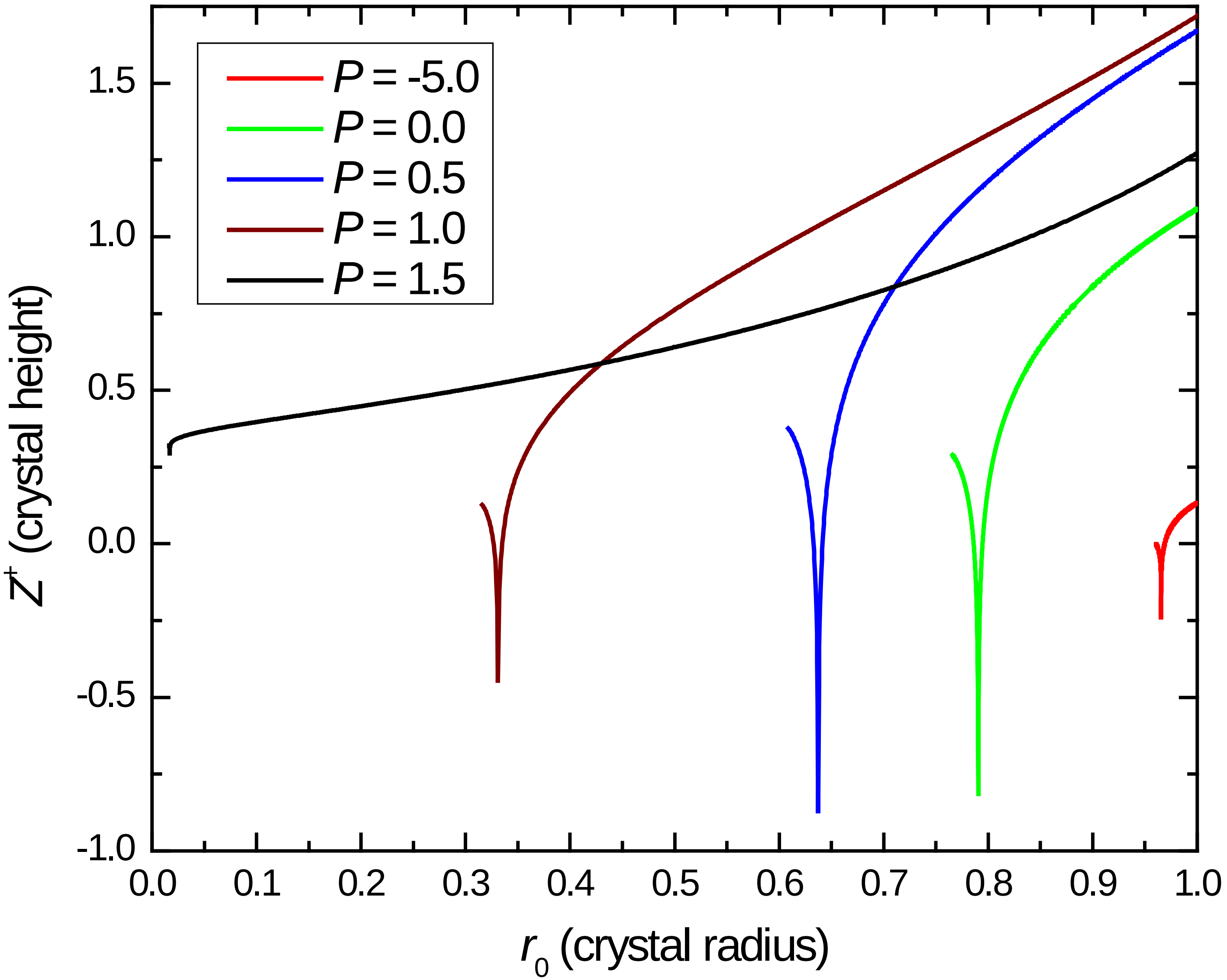
Material: Ge
Starting position, r_0: 0.6
Growth Angle: 14.3
Contact Angle: 140
ΔP = 1

Z^- : meniscus collapses when r = 0.32
Z^+: crystal eventually attaches to wall



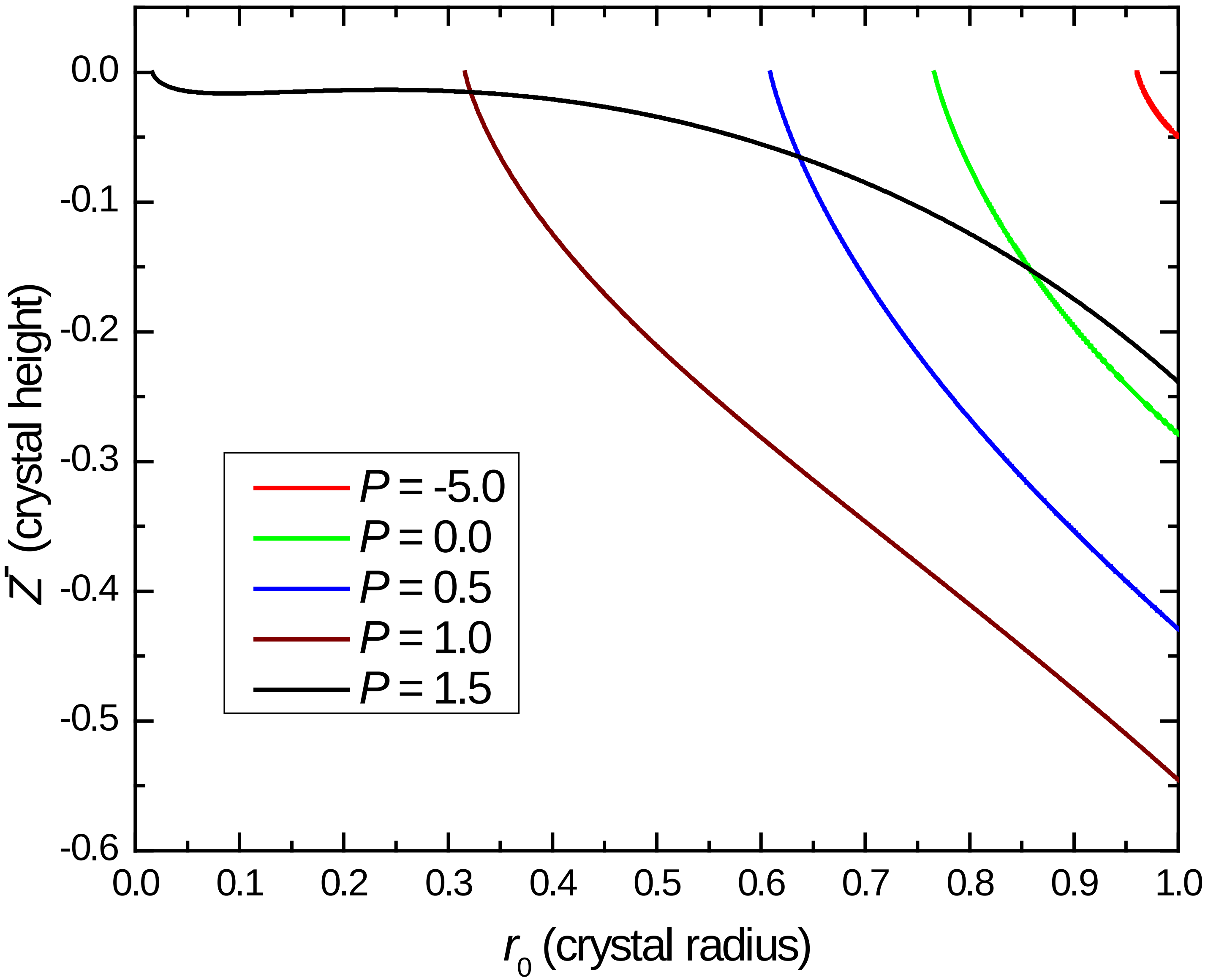
Ge Crystal Evolution for $\theta = 140$; Z^+ solution

Ge
$\alpha = 14.3$
$\theta = 140$



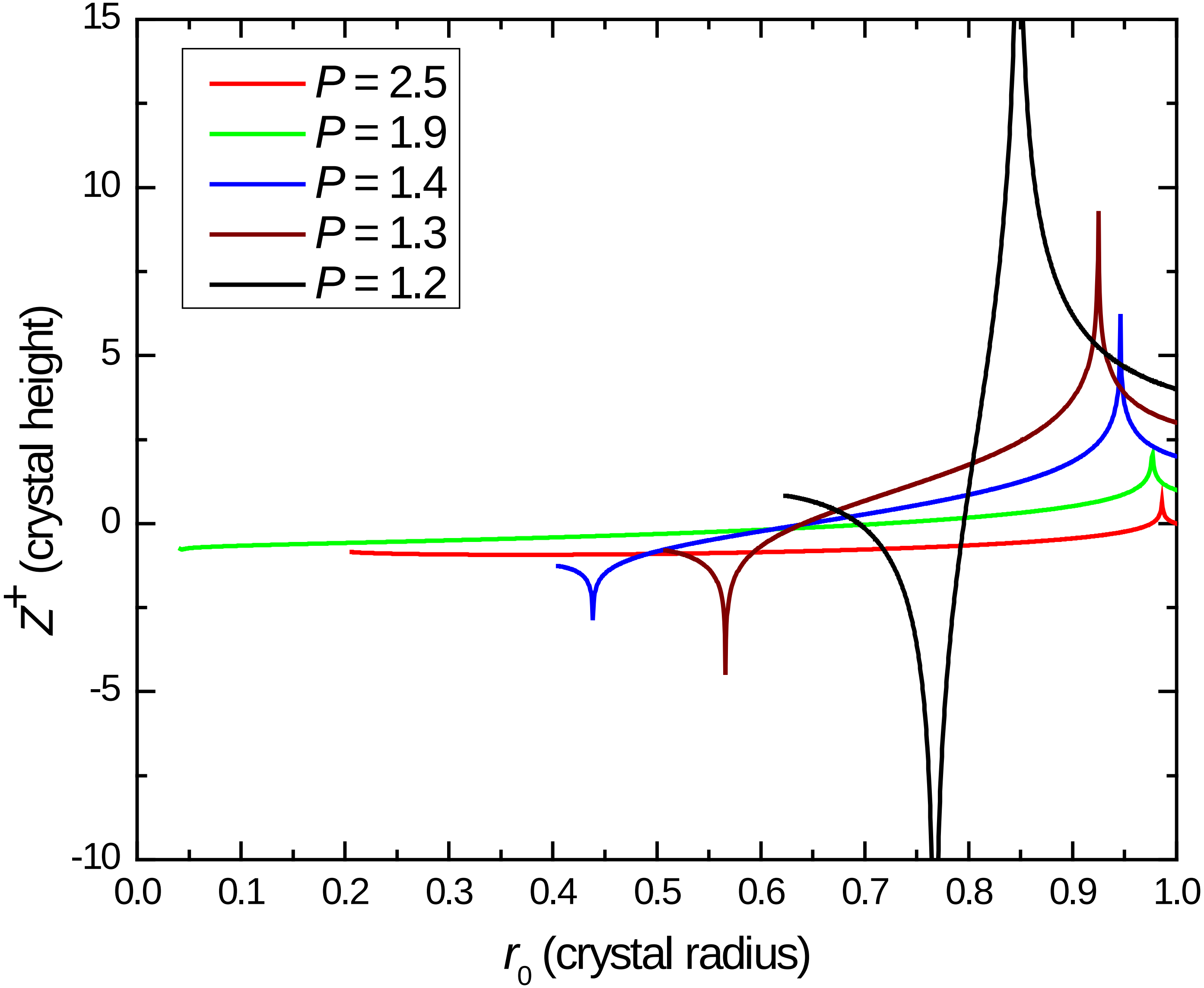
Ge Crystal Evolution for θ = 140 ; Z^- solution

Ge
α= 14.3
θ= 140



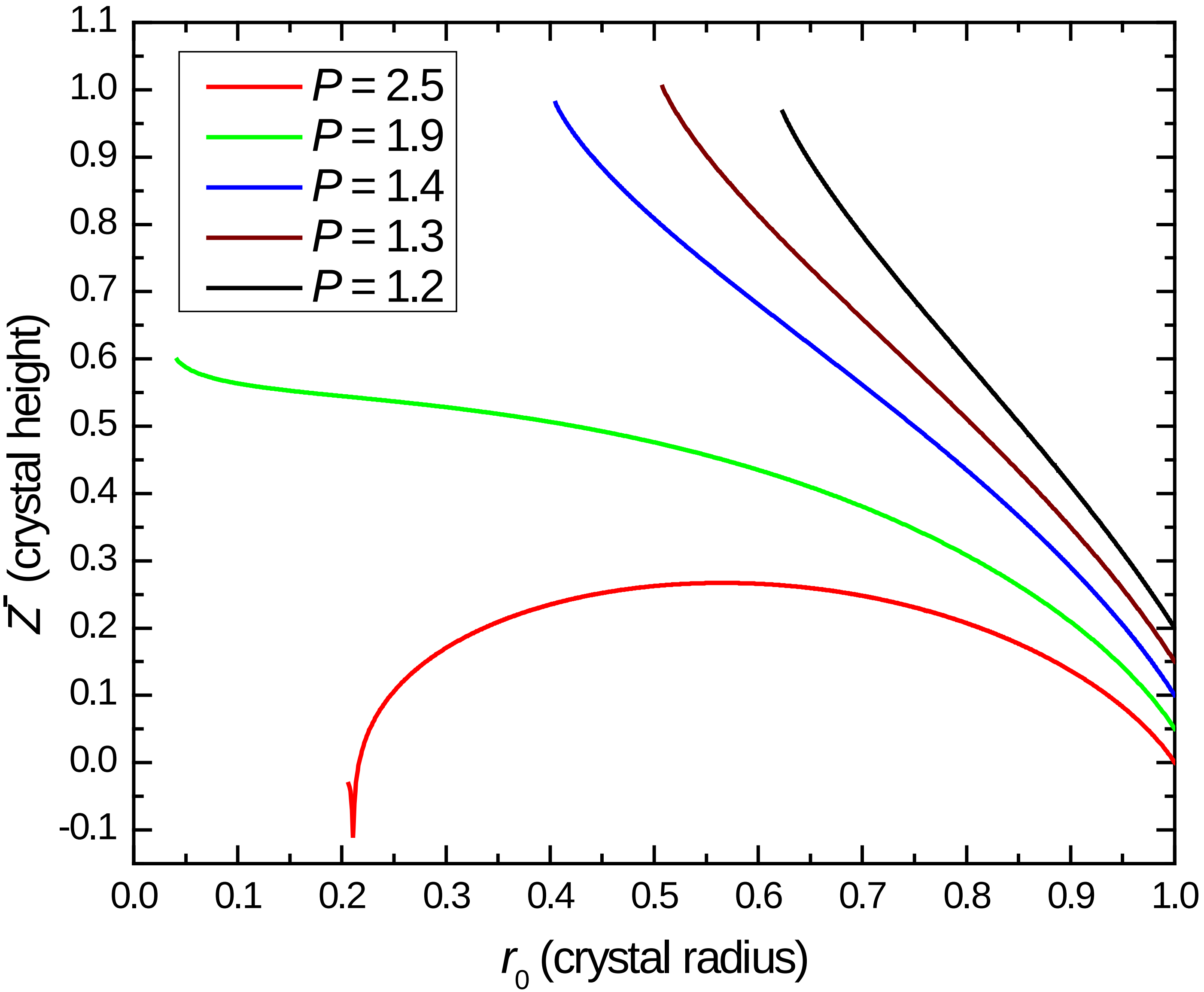
Ge Crystal Evolution for $\theta = 172$; Z^+ solution

Ge
$\alpha = 14.3$
$\theta = 172$



Ge Crystal Evolution for $\theta = 172$; Z^{-} solution

Ge
$\alpha = 14.3$
$\theta = 172$



Dynamic Stability of Crystallization

Deflection of the growing crystal radius from the stationary condition is governed by the equation

$$\delta \dot{R} = A_{RR}\,\delta R + \cancel{A_{Rh}\,\delta h}$$

In microgravity, the coefficient $A_{Rh} = 0$

Solution: $\delta R(t) = \exp\left(A_{RR} t\right)$

Dynamic stability achieved when $A_{RR} < 0$

<u>For vertical Bridgman crystal growth</u>

$$A_{RR} = -V\frac{\partial \beta}{\partial R}$$

$$A_{Rh} = -V\frac{\partial \beta}{\partial h}$$

where β is the angle between the tangential line to the meniscus and a horizontal line

V is the growth velocity

Dynamic Stability Results

$$A_{RR} = -V\frac{\partial \beta}{\partial R}$$

$$\frac{\partial \beta}{\partial R} = \frac{(\Delta PR - \cos\alpha)\sin^2\alpha}{R\sin^3\alpha - B(1-R)^2(5/24 + R/8)}$$

In microgravity, only the coefficient A_{RR} is nonzero

Therefore, dynamic stability only depends on capillarity and occurs when $\underline{\Delta P \cdot R > \cos\alpha}$

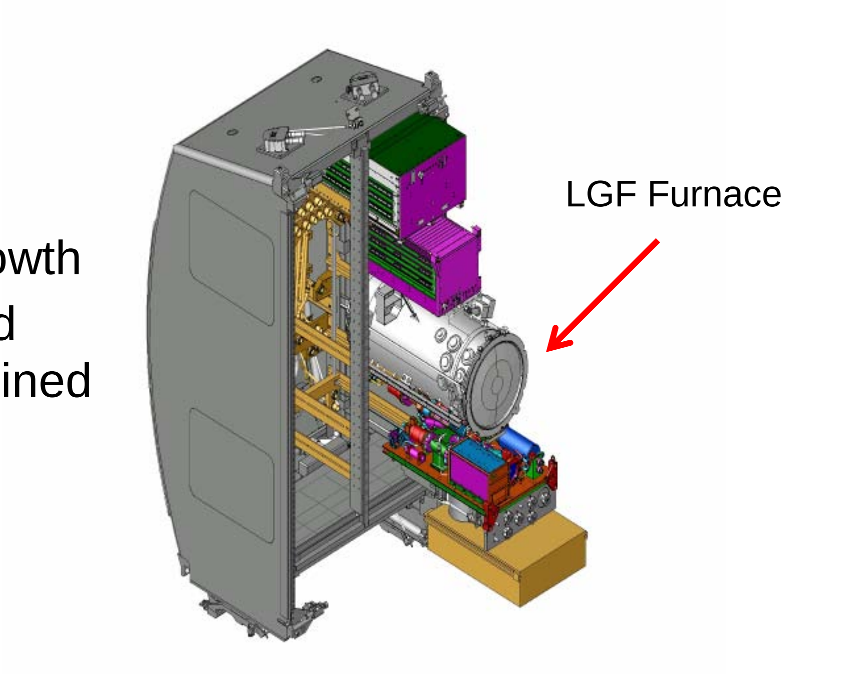
Dynamic stability calculations are in agreement with crystal evolution calculations

On Earth, dynamic stability will depend on the specific thermal conditions of the system.

ICESAGE Flight Investigation

- “Influence of Containment on the Growth of Silicon-Germanium” (ICESAGE) is a collaborative investigation between NASA and the European Space Agency (ESA)
- The ICESAGE experiments will be conducted in the Low Gradient Furnace (LGF) in the Materials Science Laboratory on the International Space Station (ISS)

- ICESAGE will test the theories of crystal shape evolution in detached Bridgman growth
- Dependence on the parameters ΔP, θ, and the crystal starting position r_0 will be examined
- Launch is currently planned on a SpaceX flight in 2015



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Summary

- A theory describing the shape evolution of detached Bridgman crystals in microgravity has been developed
- A starting crystal of initial radius r_0 will evolve to one of the following states:
  - Stable detached gap
  - Attachment to the crucible wall
  - Meniscus collapse
- Only crystals where $\alpha + \theta > 180°$ will achieve stable detached growth in microgravity
- Results of the crystal shape evolution theory are consistent with predictions of the dynamic stability of crystallization (Tatarchenko, *Shaped Crystal Growth*, Kluwer, 1993)
- Tests of transient crystal evolution are planned for ICESAGE, a series of Ge and GeSi crystal growth experiments planned to be conducted on the ISS