Shape Evolution of Detached Bridgman Crystals Grown in Microgravity
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)?
Detached Crystal Growth
Schematic Diagram of Detached Solidification

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

$$\Delta P = \Delta P_{\text{external}} + \rho gh + 2 \frac{\gamma}{r_{tm}}$$

where

- $\Delta P_{\text{external}}$: external gas pressure differential
- $\rho gh$: weight of melt (pressure head)
- $2 \frac{\gamma}{r_{tm}}$: capillary pressure from top meniscus
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

\[ \frac{dZ^\pm}{dr} = \frac{\sqrt{4r^2 - y^2} \tan \alpha \pm y}{\sqrt{4r^2 - y^2} \mp y \tan \alpha}, \quad y = \Delta P(r^2 - 1) - 2 \cos \theta \]
Crystal Evolution for $\theta + \alpha > 180^\circ$; $Z^+$ solution

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

$Z^+$ (crystal height)

$r_0$ (crystal radius)
Ge Crystal Evolution for $\theta + \alpha > 180^\circ$; $Z^+$ solution

Material: Ge
Growth Angle: 14.3°
Contact Angle: 172°
$\Delta P = 1.4$

(a) Radius decreases until meniscus collapses

(b, c) Radius increases or decreases until stable growth with a constant radius is reached
Ge Crystal Evolution for $\theta + \alpha > 180^\circ$; $Z^-$ solution

Material: Ge
Growth Angle: $14.3^\circ$
Contact Angle: $172^\circ$

For $Z^-$ solutions, all crystals decrease in radius until the menisci collapse.
Existence Region for $\theta + \alpha > 180^\circ$
Crystal Evolution for $\theta + \alpha < 180^\circ$

$Z^+$ solutions

$Z^-$ solutions

$\alpha = 14.3^\circ; \theta = 140^\circ$
Crystal Evolution for $\theta + \alpha < 180^\circ$

Material: Ge  
Growth Angle: 14.3°  
Contact Angle: 140°  
$\Delta P = 1.0$

(a, c) Radius decreases until meniscus collapses

(b) Radius increases or decreases until attachment at the crucible wall
Existence Region for $\theta + \alpha < 180^\circ$

- $\frac{dr}{dZ} = 0$; unstable
- $\frac{dr}{dZ} \neq 0$
- no solution

$\theta = 140^\circ$
$\alpha = 14.3^\circ$
“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 $\Delta P$, $\theta$, and the crystal starting position $r_0$ will be examined.

Launch is currently planned on a SpaceX flight in 2016.
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 $\alpha + \theta > 180^\circ$ 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