Materials Science in Space: Preparation of Bulk Semiconductors and Photovoltaic Materials

Materials in Space Workshop

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170mm diameter Silicon crystal for 125mm "pseudo-square" solar cell; similar to 150mm diameter for Semiconductor

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Why desire "large" single crystals?

- Most parts made from metals and alloys and ceramics are composed of many small single-orientation grains bound to each other with random relative orientation
- There are reasons why a "single crystal" can be desired for certain applications
  - Highly uniform macroscopic properties (3D lattice)
  - Anisotropic properties
  - Energy-Momentum Relationship/Band/Electronic States
  - Grain boundaries degrade function/properties
- *Solidification* is a desirable crystal growth process because of relatively high phase transformation rate (cost) and ability to use temperature to affect driving force (Gibbs Free Energy or gradient of chemical potential). *Vapor transport growth* is also used for non-congruently melting compounds. *Solution growth* also sometimes used.

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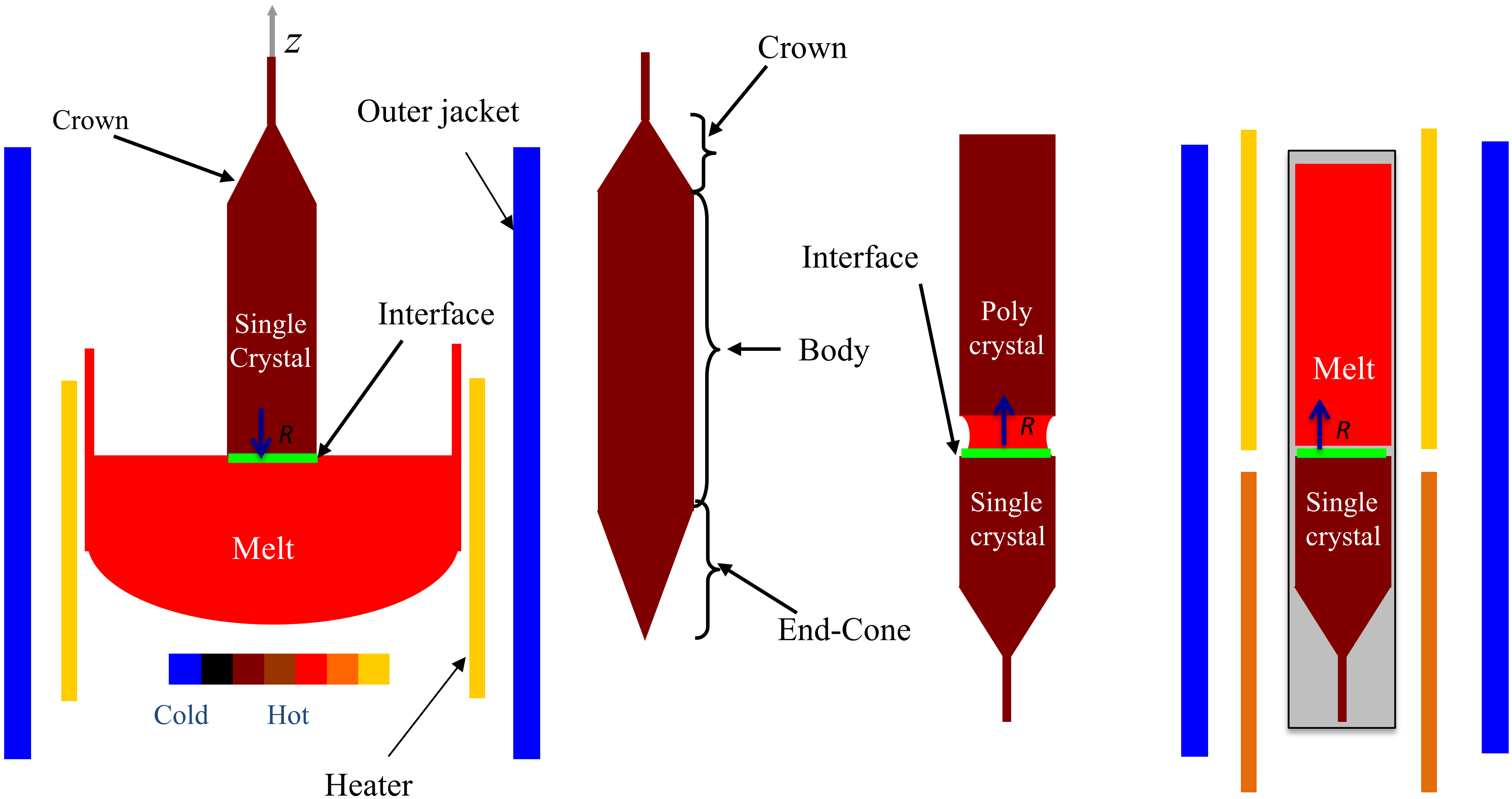
Directional Solidification Processes to Grow Single Phase Single Crystals



Czochralski (Cz) Process (Teal & Little)

Cz Crystal

Float Zone Process (Pfann)

Bridgman-Stockbarger Process

(variations: “HEM”, “Gradient Freeze”)

Traditional Interest in using "space"

- Reduced Body Acceleration Field ("microgravity")
  - Buoyancy Driven Convective Mass and Heat Transfer
    - Segregation
    - Melt thermo-physical property determination
    - solute gradient, temperature gradient stability
    - Masked phenomena (e.g. thermocapillary flows)
  - Container Contact
  - Hydrostatic Pressure
  - Sedimentation and Stokes Flows
- Other unique environment effects
  - Vacuum (use for epitaxial layer growth – MBE/ALE)

Doped Elements: Si, Ge

Doped Compounds: GaAs, CdTe, InP, SiC…

Undoped Compounds: GaN, AlN, AlSb…

Ternaries (i.e., CdZnTe, HgCdTe, PbSnTe, GaInAs)

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Segregation Studies (InSb)

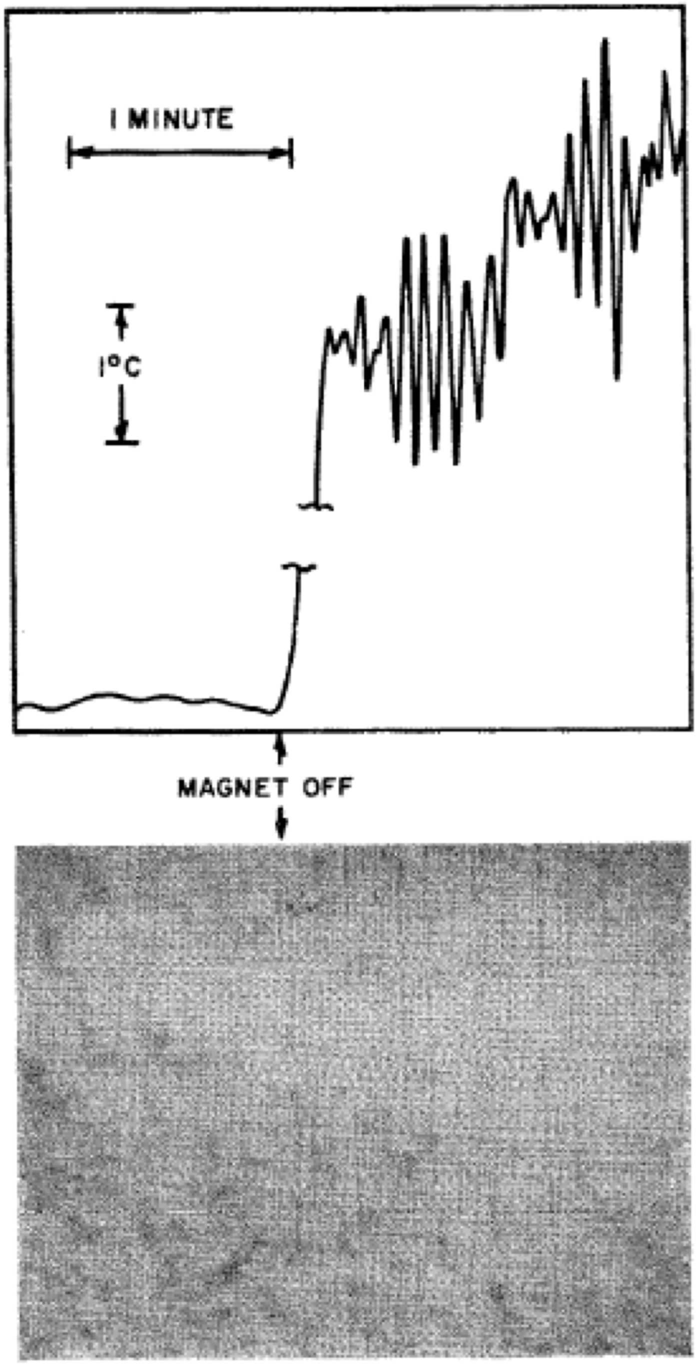
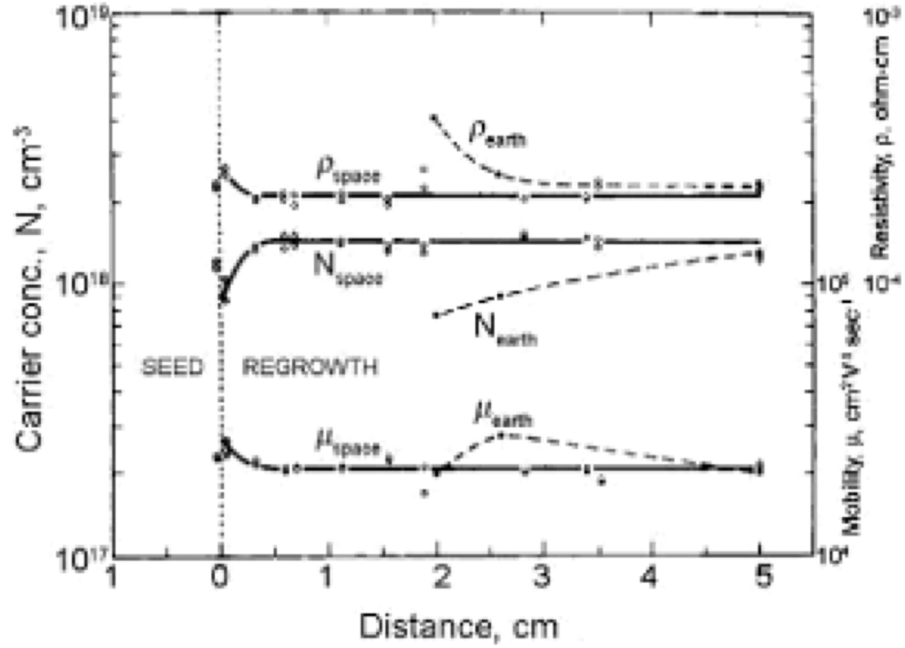


FIG. 2. Run No. 1. The direction of growth is from left to right in both photomicrograph (×150) and recorder trace.



A. F. Witt, H. C. Gatos, M. Lichtensteiger, M. C. Lavine and C. J. Herman, "Crystal Growth and Steady-State Segregation under Zero Gravity: InSb", J. Electrochem. Soc. 1975 volume 122, issue 2, 276-283.

Harvey P. Utech and Merton C. Flemings, "Elimination of Solute Banding in Indium Antimonide Crystals by Growth in a Magnetic Field", Journal of Applied Physics 37, 2021 (1966).

Segregation Studies (Ge)

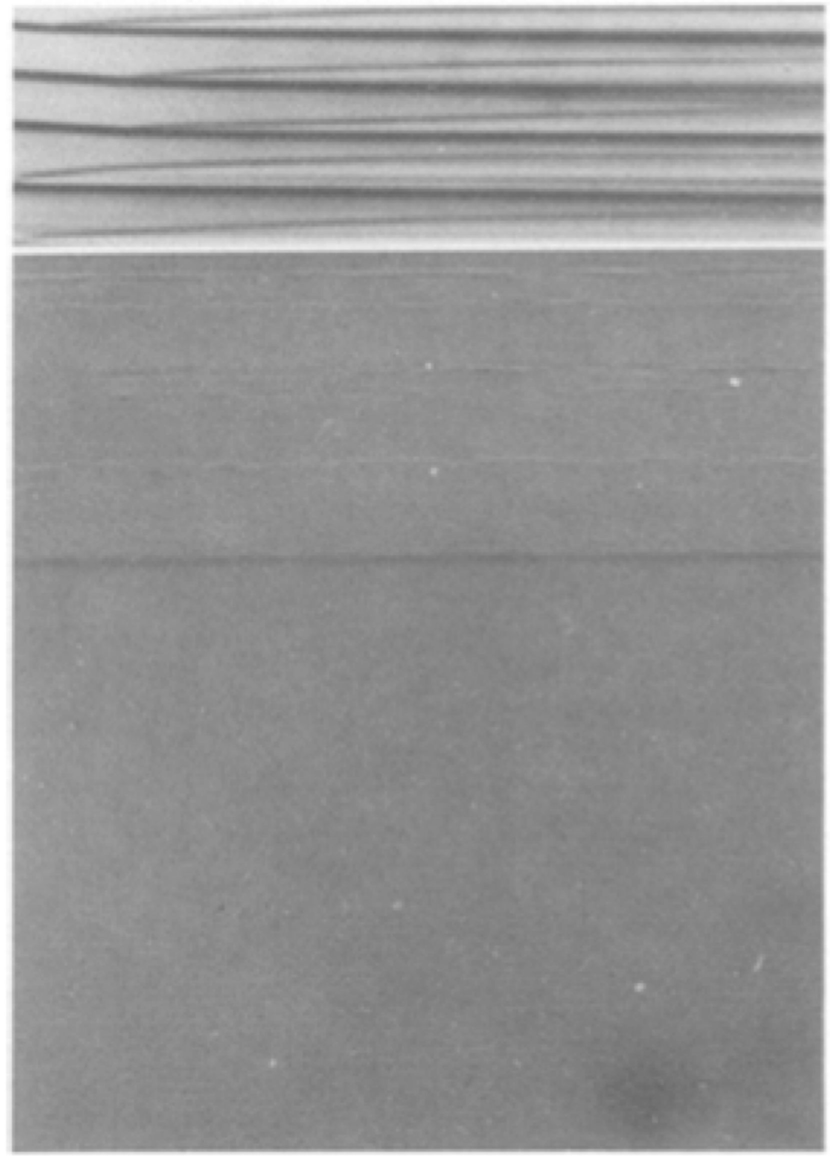


Fig. 7. Segment of Ge crystal partially regrown in space: note seed segment (top) and segment of controlled regrowth (bottom) separated by a region of uncontrolled growth and segregation.

A. F. Witt, H. C. Gatos, M. Lichtensteiger and C. J. Herman, J. Electrochem. Sot.: Solid-State Science And Technology, November 1978, 1832-1840.

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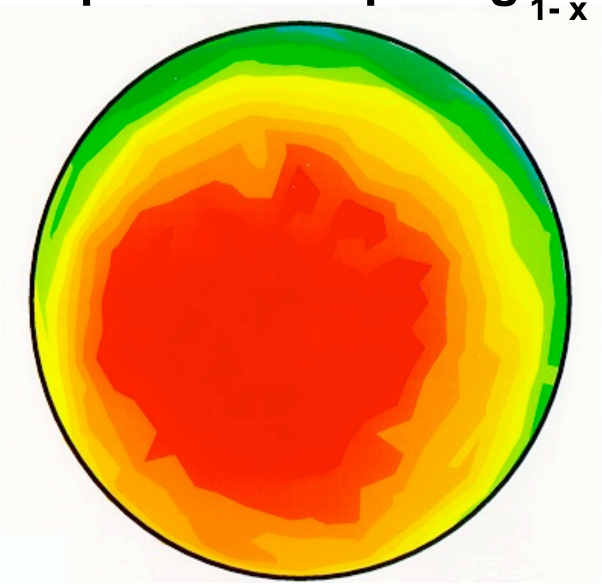
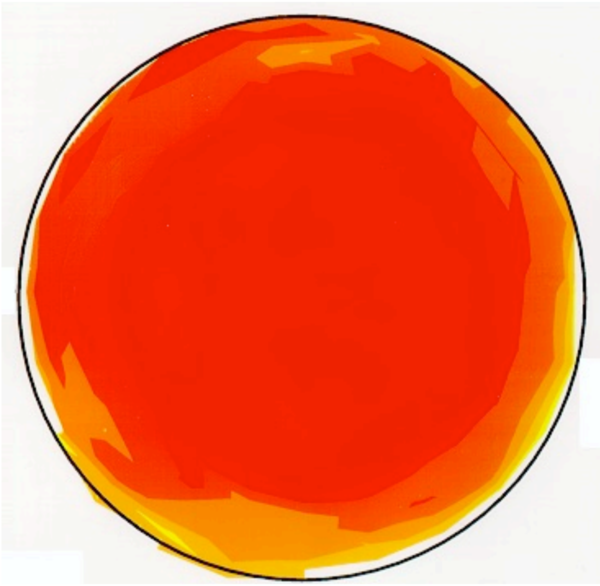
Segregation Studies (HgTe-CdTe)

GROWTH OF SOLID SOLUTION SINGLE CRYSTALS
P.I. Sandor L. Lehoczky, Marshall Space Flight Center

Composition Maps $Hg_{1-x}Cd_xTe$



Earth Test in Furnace



Microgravity Result (STS-62)

Convection on Earth caused by radial temperature gradients results in large inhomogeneities of composition, even if thermo-solutally stabilized normal to growth. In microgravity this convection is reduced and the material is more uniform

Application : bulk infrared sensor - must be homogeneous

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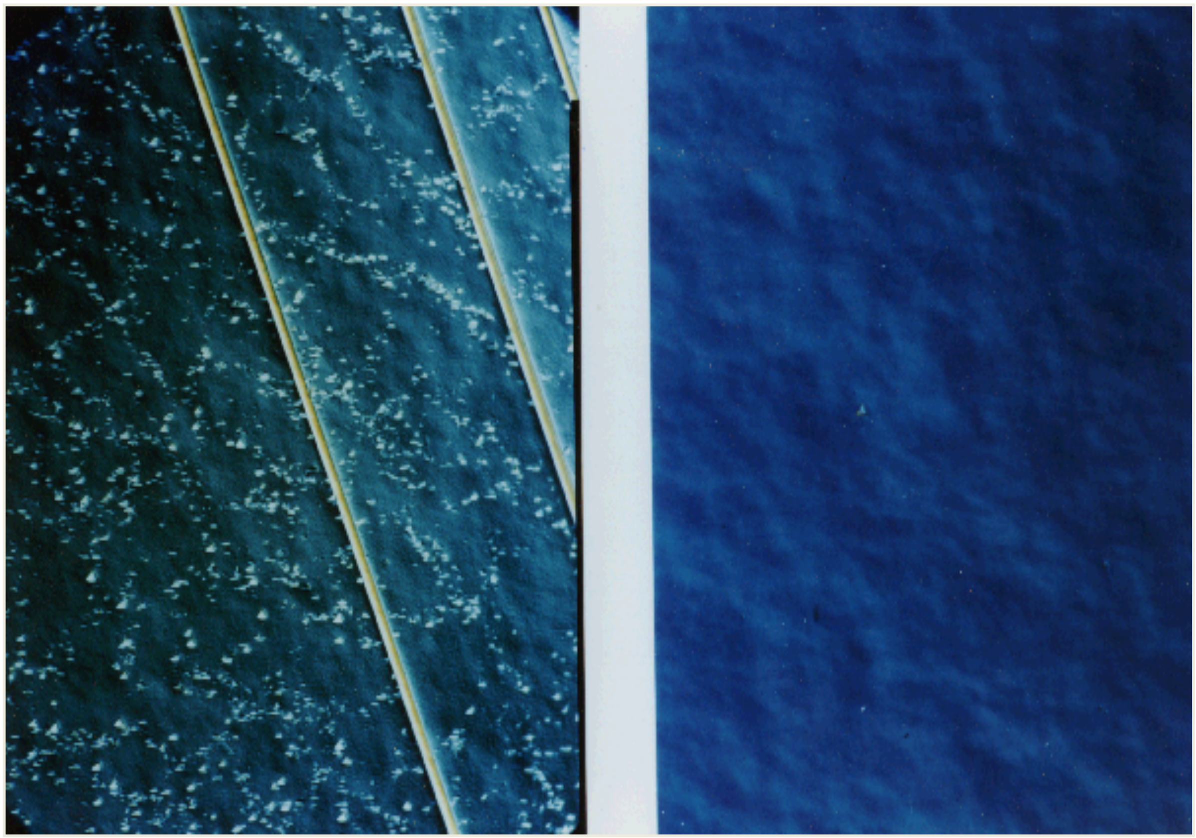
Structural Defect Studies (CdZnTe)

ORBITAL PROCESSING OF HIGH-QUALITY Zn-alloyed CdTe COMPOUND SEMICONDUCTORS

P.I. David L. Larson, Jr., SUNY-Stony Brook

Ground Test: Shows high area density of etch pits (dislocations) and twin lamella (growth stacking faults)



Microgravity Result (STS-50): Shows reduced etch pit count, fewer twins

Shows Effect of Container Contact, Hydrostatic Pressure

Fewer Defects in Microgravity may be due to:

1) "Detached solidification" - no wall contact;

2) No force on solid material immediately following solidification

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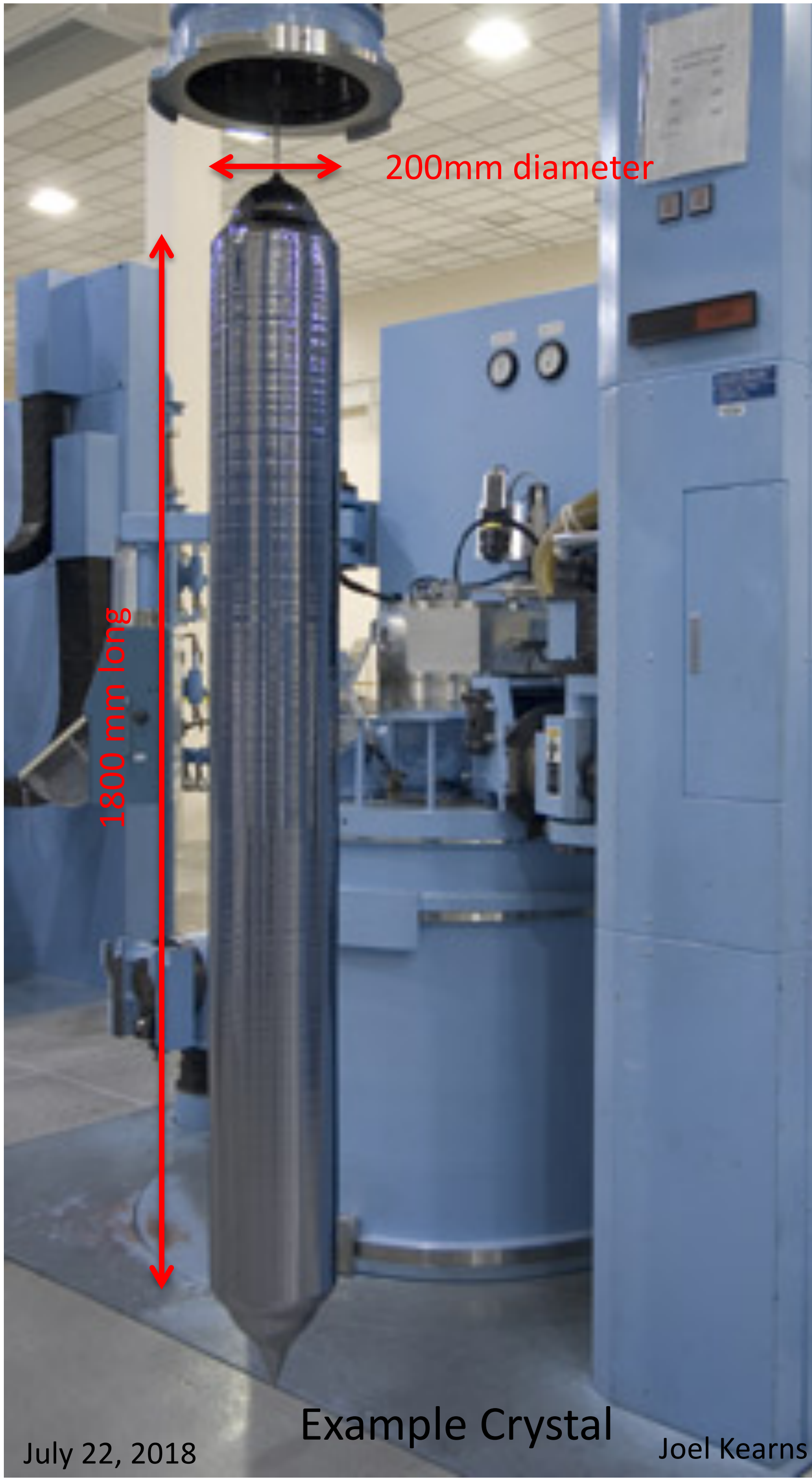
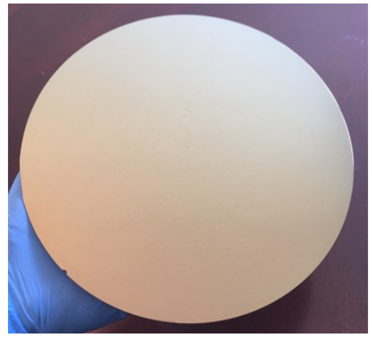
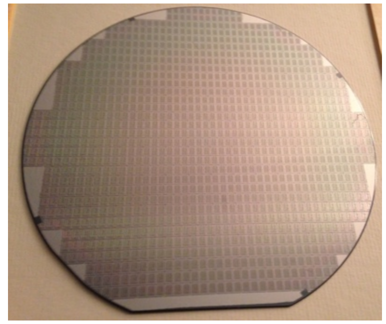


Example Crystal

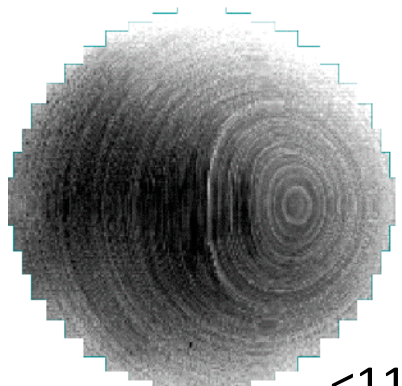


Wafer is cut from crystal



Chips are made in Wafer

But...



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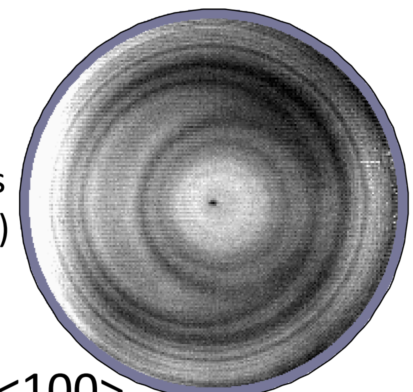
Impurities distribution affects Chips (Segregation)



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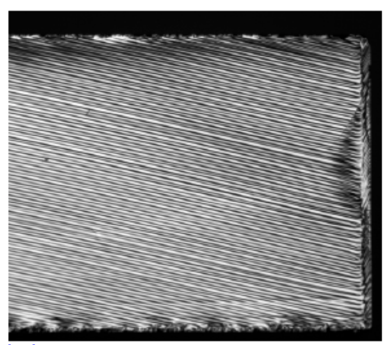

Impurities distribution both across and through wafer

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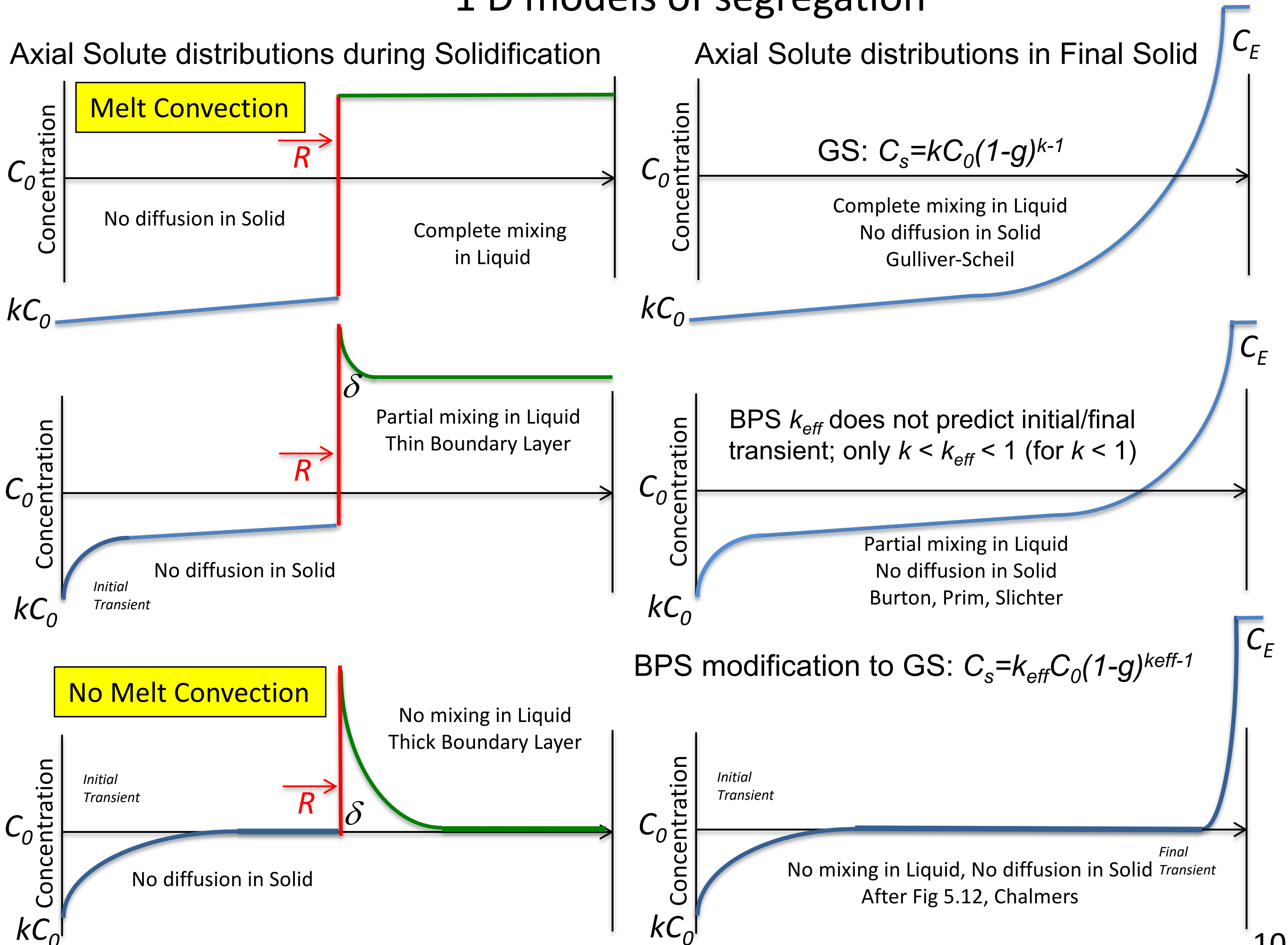
1 D models of segregation



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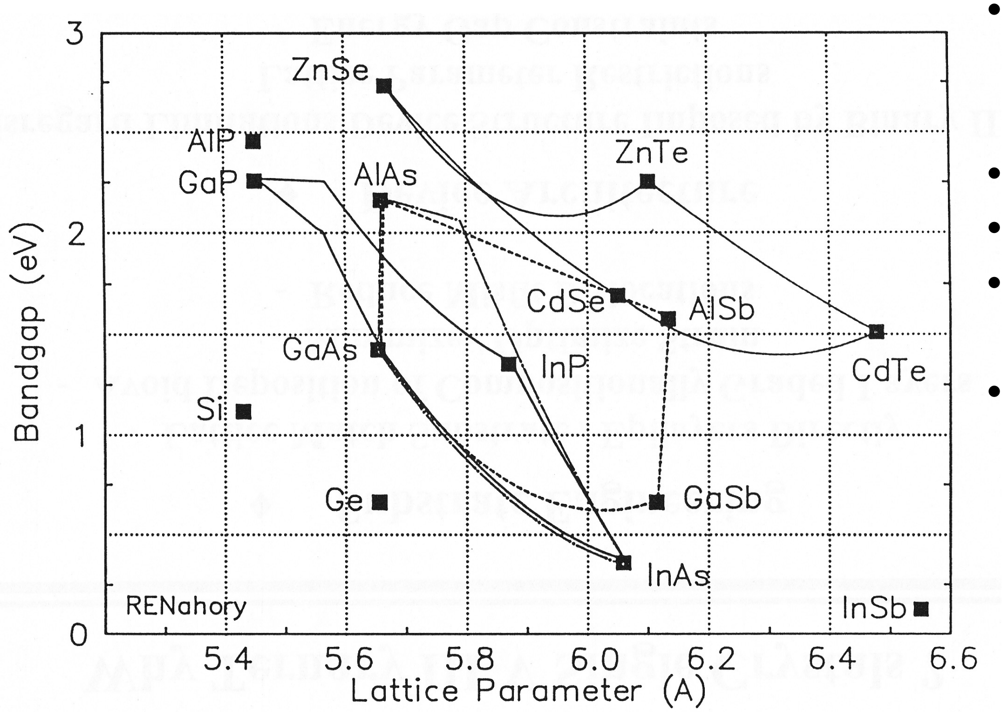
Ternary III-V Crystals



Problems from varying Composition / Lattice Parameter along crystal length

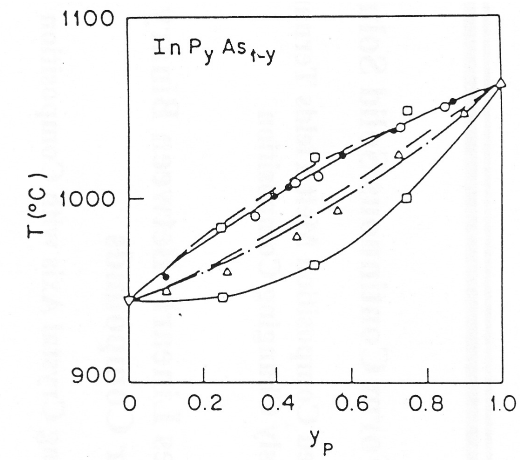
- Stress
- Cracking
- Cellular Interface leading to Polycrystal
- Twinning
- Electrical Characteristics
- Fabrication/Polishing
- Growth Process

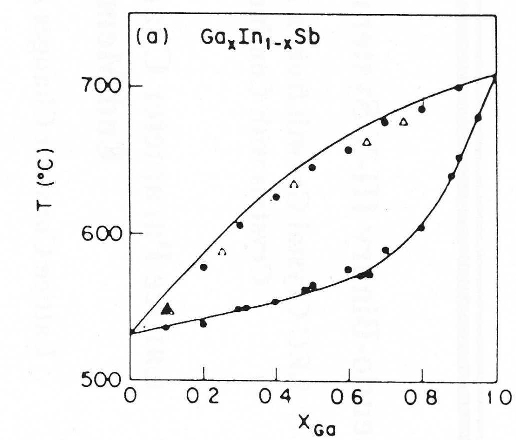
Use of Ternary Substrate:

- Lattice Match Substrate to epitaxially grown Layer for device region
- Avoid graded layer deposition
- Minimize/Optimize Strain
- Reduce device region misfit dislocations
- Novel bulk devices

Potential Devices:

- GaInAs: ZnSe Blue Emitter; pHEMT > 2 GHz
- GaInP: Visible Emitter
- InPAs: mid-IR Laser
- GaInSb: Sb Laser > 3 um; IR detector
- InAsSb: Mid-IR 3-5um windows





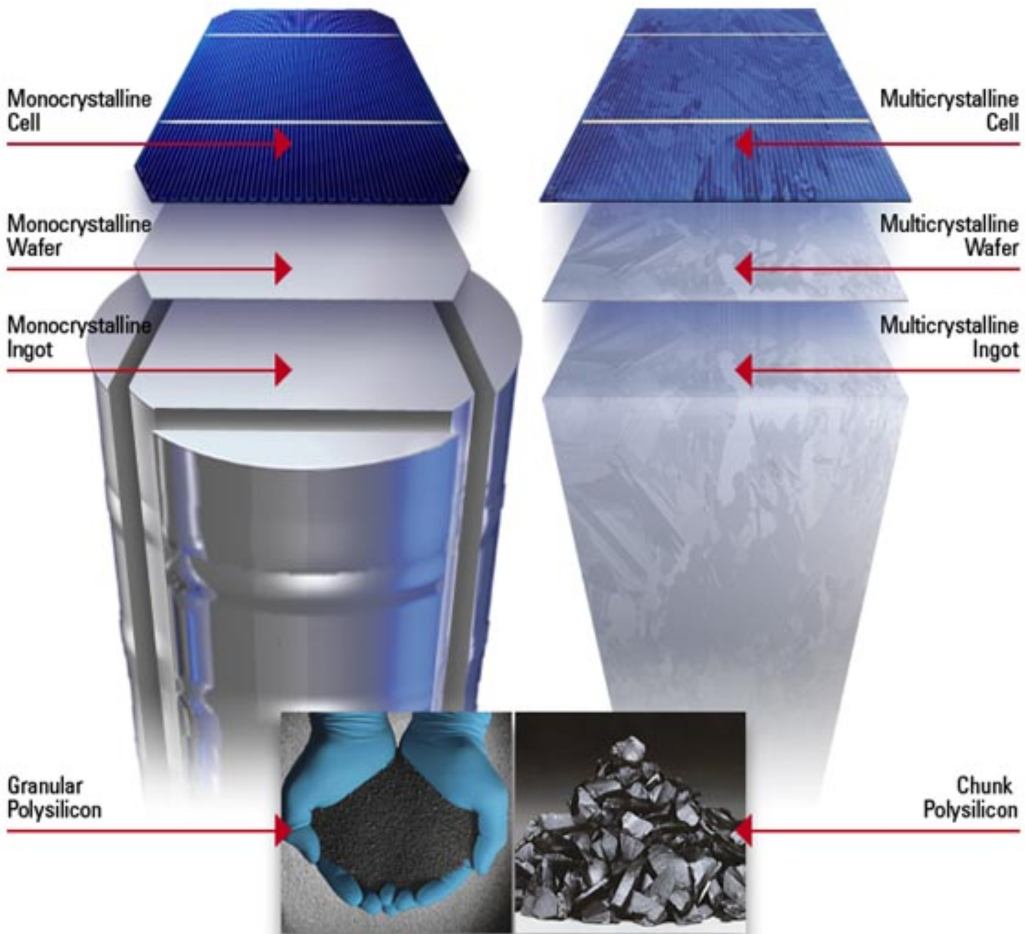
W. Bonner, "Bulk Ternary III-V Single Crystals: Growth and Characterization", 11th American Conference on Crystal Growth and Epitaxy (1999) Vail, Colorado.

Bachmann et. al., *Progress in Crystal Growth and Characterization*, Pergamon Press, Vol 2 (1979)

Silicon Wafers for Solar Cells on Earth – “mono” & “multi”

Standard “Mono” Characteristics

- P-type
- Pulled by Cz technique
- Resistivity ~ 0.5-3ohm-cm
- Nominal thickness ~ 160-190um
- Oxygen < ~ 10-18ppma
- Carbon < ~ 1ppma
- Nitrogen – none
- Secondary Phases - none
- Threading Dislocation-free
- Lifetime > 10usec on block
- Passivated lifetime > 150 usec (on slice)
- LID ~ high
- single orientation (100) = lower reflectivity texturing
- AlBSF Cell Efficiency ~ 19.5+%; PERC ~ 20+%



Standard “Multi” Characteristics

- P-type
- Directionally Solidified by Gradient Freeze technique
- Resistivity ~ 0.5-3ohm-cm
- Nominal thickness ~ 180-200um
- Oxygen < ~ 8 ppma
- Carbon < ~ 7 ppma
- Nitrogen (saturated)
- Secondary Phases present
- Dislocations ~ E5/cm2
- Lifetime > 2usec on block
- Passivated lifetime > 10 usec (on slice)
- LID ~ low
- multi orientation = higher reflectivity texturing
- AlBSF Cell Efficiency ~ 17.5%

- Unlike Semiconductor, no drive to greatly increase diameter, as solar cells are “whole wafer” device of industry standard size. 156mm “PS” requires ~200mm diameter crystal
- Sometimes “full square” wafer

From J. Kearns, J. Holzer, R. Nandan, J. Binns and E. Good, “N-type Mono CZ Silicon: Continuous Czochralski Silicon for high efficiency n-type solar cells”, 23rd Workshop on Crystalline Silicon Solar Cells & Modules: Materials and Processes, July 28 2013

1650 KG multicrystalline Silicon ingot
for mc-Si cells

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"Today's" Challenges: CZ for Si Semiconductors & PV

Semiconductor Si:

- International Technology Roadmap for Semiconductors shows path
- 300mm for < 5 nm site flatness and new device structures
- Bulk crystal composition contributions to 3D device structures
- 450mm diameter – when?
  - Crystal microdefects
  - Will new device structures demand new micro-defect or segregation engineering, or impurity reductions?
- R&D for next diameter increase: 675mm?

PV Si:

- Crystal & Wafer component of $/Wp
  - Conversion cost, poly cost
  - Efficiency
- Minority Carrier Lifetime (MCLT) distribution crystal to crystal and within crystals for advanced cell architectures
- International Technology roadmap for Photovoltaics (ITRPV)
- Next Generation Materials: any real advantage?

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Opportunities for Materials Science in Space

- For bulk semiconductors, crystal mass, size and power / cooling to solidify dominate discussions: is there power to grow needed size?
- Fluid convection is not always "bad"

Bulk Semiconductors:

- Testing of processing – structure relationships for Earth-based process simulation (Materials Science investigations)
- "Uniform" axial and radial composition ternaries for lattice matched substrates for advanced electro-optic devices
- Reduced structural defects in "soft" semiconductors (i.e., detached crystal growth to avoid container interactions during directional solidification)
- Determination of thermo-physical properties for Earth-based process simulation
- Preparation of "existence proof" samples for structure / properties benchmarks – a reference state of matter - standards

Photovoltaics:

- ISRU – can PV cells be made in space from available resources?
- Understanding "next generation" PV materials systems processing-structure-properties relationships (perovskites, organics)

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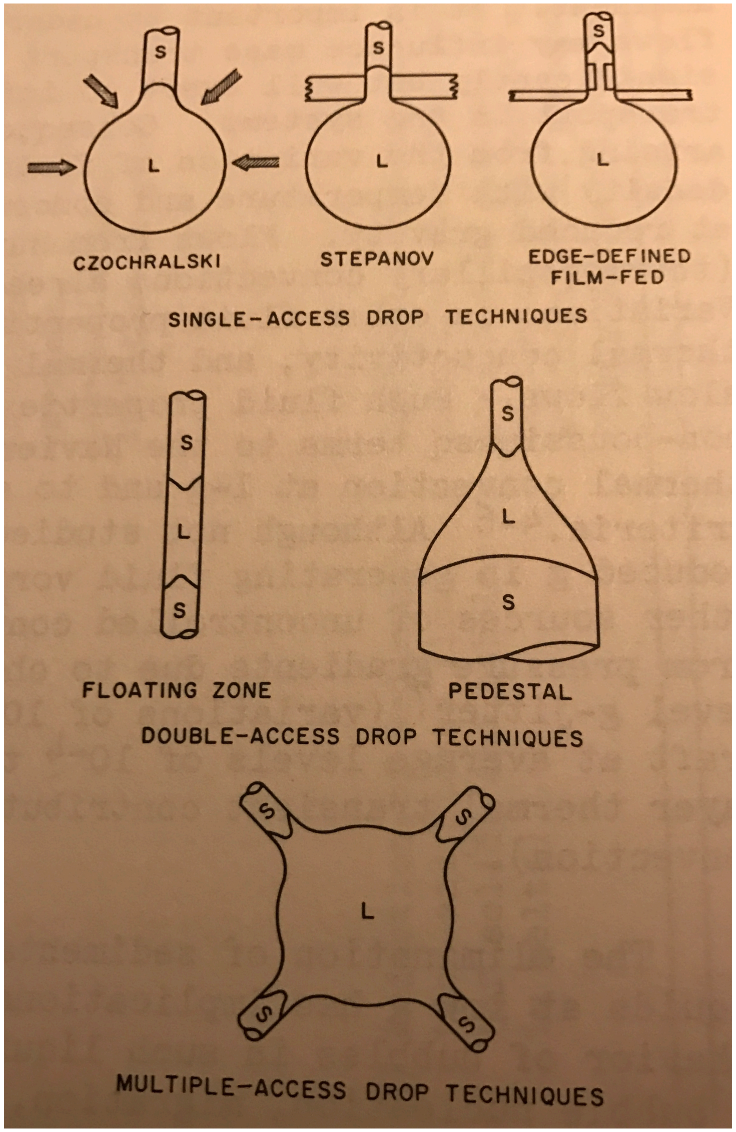
Potential Crystal Growth Processes to more fully exploit the Microgravity Environment



J. R. Carruthers, "The application of drops and bubbles to the science of space processing of materials", in International Colloquium on the Science of Liquid Drops and Bubbles, Edited by J. Collins, JPL, Pasadena (1976).

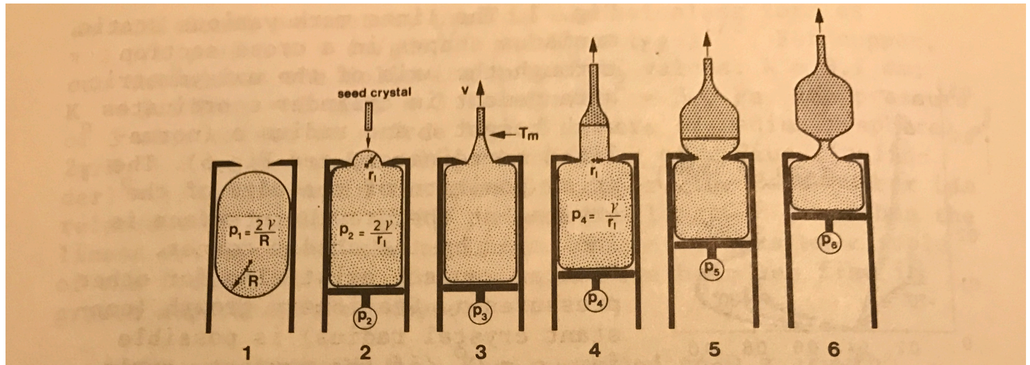


Fig. 9 Crystal growth in 0 g by Czochralski method. Sequence of typical moments: 1) Cylindrical container with nonwetting melt. 2) Piston induces increased hydrostatic pressure until maximum pressure is reached when melt is protruding as hemisphere out of circular hole in mask with radius r_1. 3) Contact with seed crystals is established at isotherm T_m of the melting temperature (increasing temperature in downward direction). The crystal diameter increases during further growth with pulling speed v. The meniscus shape can be changed by varying either p_3 or position of isotherm T_m. 4) Cylindrical meniscus shape is possible only for a specific pressure $p_4 = \gamma/r_1$ ("bottleneck" in growth sequence as far as freedom of choice of pressure is concerned). 5) Decrease of crystal diameter. 6) Further decrease of crystal diameter (beginning of necking or end of growth process).

H. Wenzl, "Czochralski Growth of Crystals in 0-g and 1-g", COSPAR Symposium on Materials Sciences in Space, Philadelphia, Pennsylvania (1976).

Kearns' Back-up

Materials Science in Space:

Preparation of Bulk Semiconductors and Photovoltaic Materials

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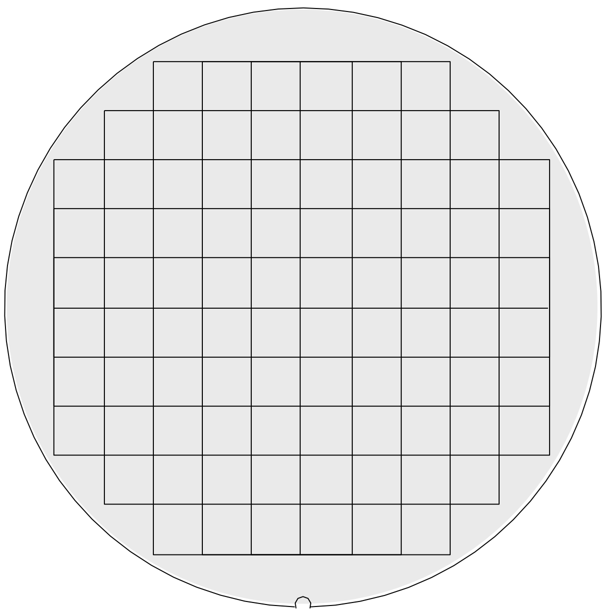
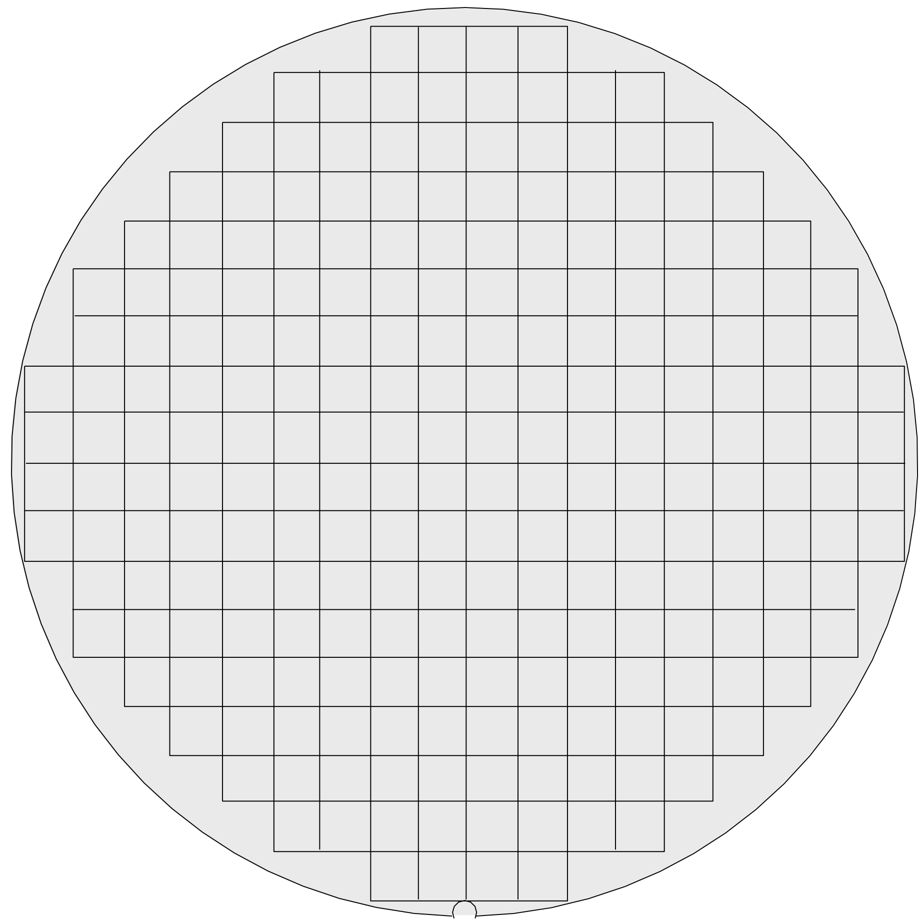
Increase in Number of Chips using Larger Diameter Silicon Wafers

(Assuming large 1.5 x 1.5 cm microprocessors)



88 die

200-mm wafer



232 die

300-mm wafer

Wafer scale-up and transistor critical dimension reduction enable increased functionality and lower cost

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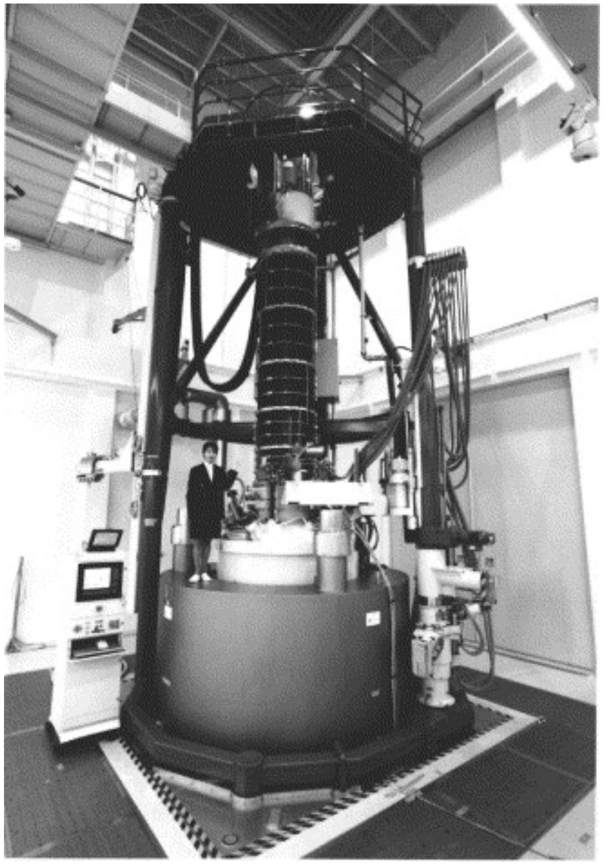
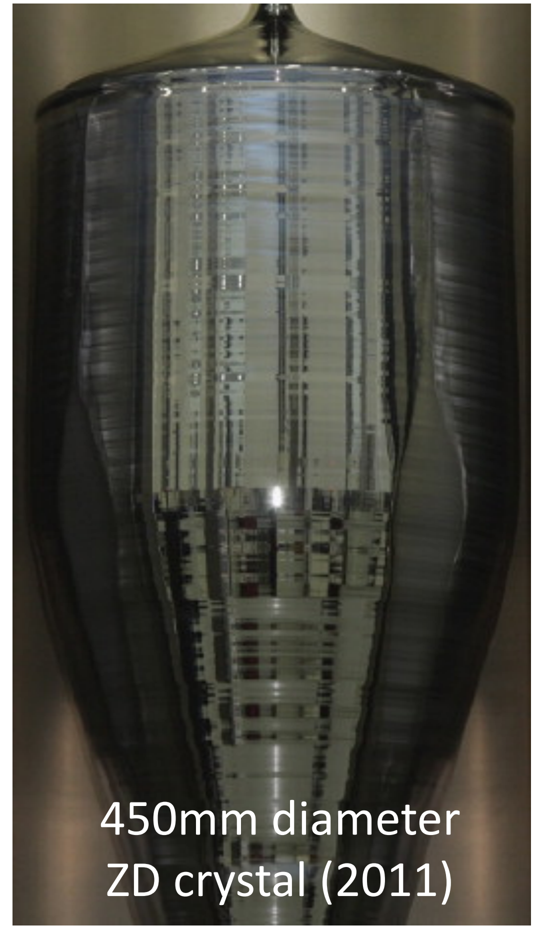
400mm-450mm Diameter Silicon



"Super Silicon" Puller

400mm diameter DF crystal



450mm diameter ZD crystal (2011)

300mm vs. 450mm slice

From "Growth of silicon crystal with a diameter of 400mm and weight of 400 kg" Y. Shiraishi*, K. Takano, J. Matsubara, T. Iida, N. Takase, N. Machida, M. Kuramoto, H. Yamagishi, Journal of Crystal Growth 229 (2001) 17–21.

From "Growth of 450mm diameter semiconductor grade silicon crystals", Zheng Lu and Steven Kimbel, Journal of Crystal Growth, Volume 318, Issue 1, 1 March 2011, Pages 193-195.

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Impact of D-defects (COPs) on Devices – leakage & GOI

LOCOS isolation failure

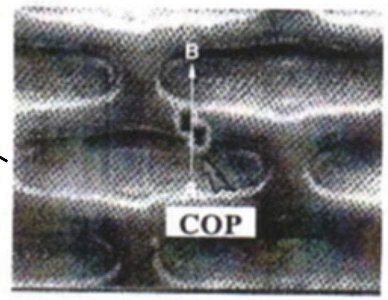


Fig.13 COP induced isolation failure in a DRAM device.

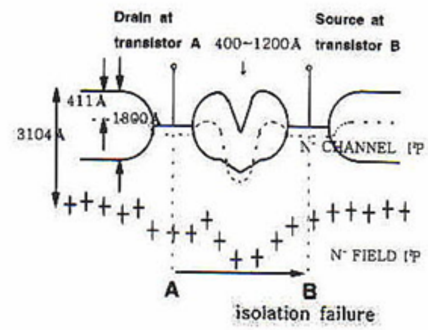


Fig.15 COP induced isolation failure

Isolation failure in a DRAM device showing sensitivity to the size of the COP, larger COPs higher probability of isolation failure

Reference: Park, et. al, ECS conf. On Defects in Silicon, Seattle, Washington. May 1999.

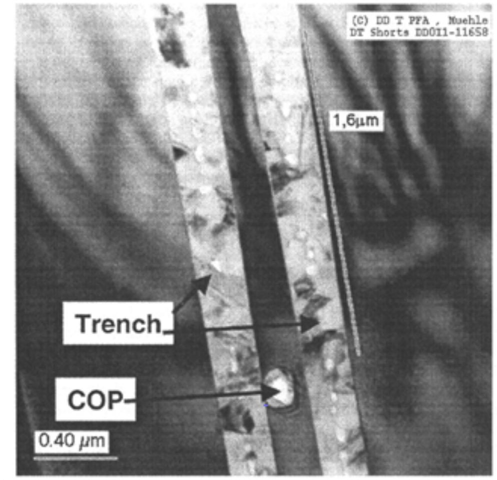


Figure 6. Scanning electron microscope (SEM) image of a COP short fail between adjacent deep trenches of an actual fabricated DRAM product, clearly showing the storage dielectric and poly electrode fill and the empty space in the COP center. Trenches are located above and below the photograph level.

COP-free depth and COP density/size important for deep trench capacitors on DRAM or eDRAM

Deep trench leakage

E. Dornberger, et. al, J. Electrochem. Soc., 149 (4) G226-231 (2002).

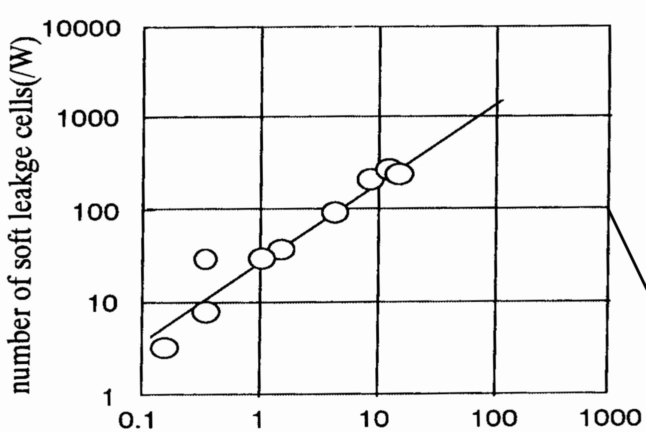


Fig.6.Correlation between the number of soft leakage cell and LSTD density

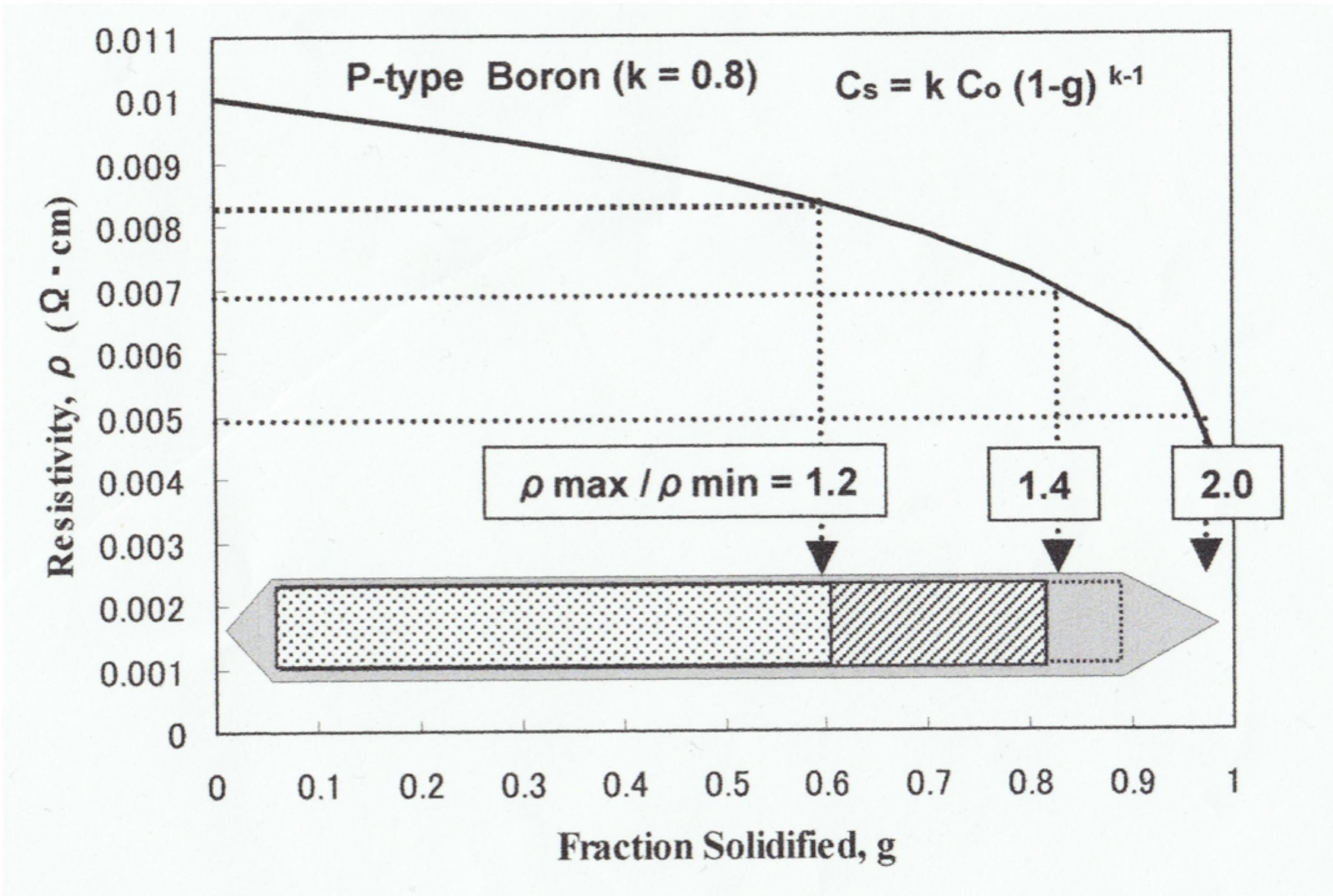
Ref: Kubota, et al, ECS PV2000-17.

Device leakage failures

Smaller features demand small structure control; but structure is derived from solid-state transformations, which are not affected by gravity

Resistivity in Cz Silicon Crystal

Resistivity range effect on Yield: Boron dopant



Customer specification of resistivity range can greatly affect crystal yield and cost

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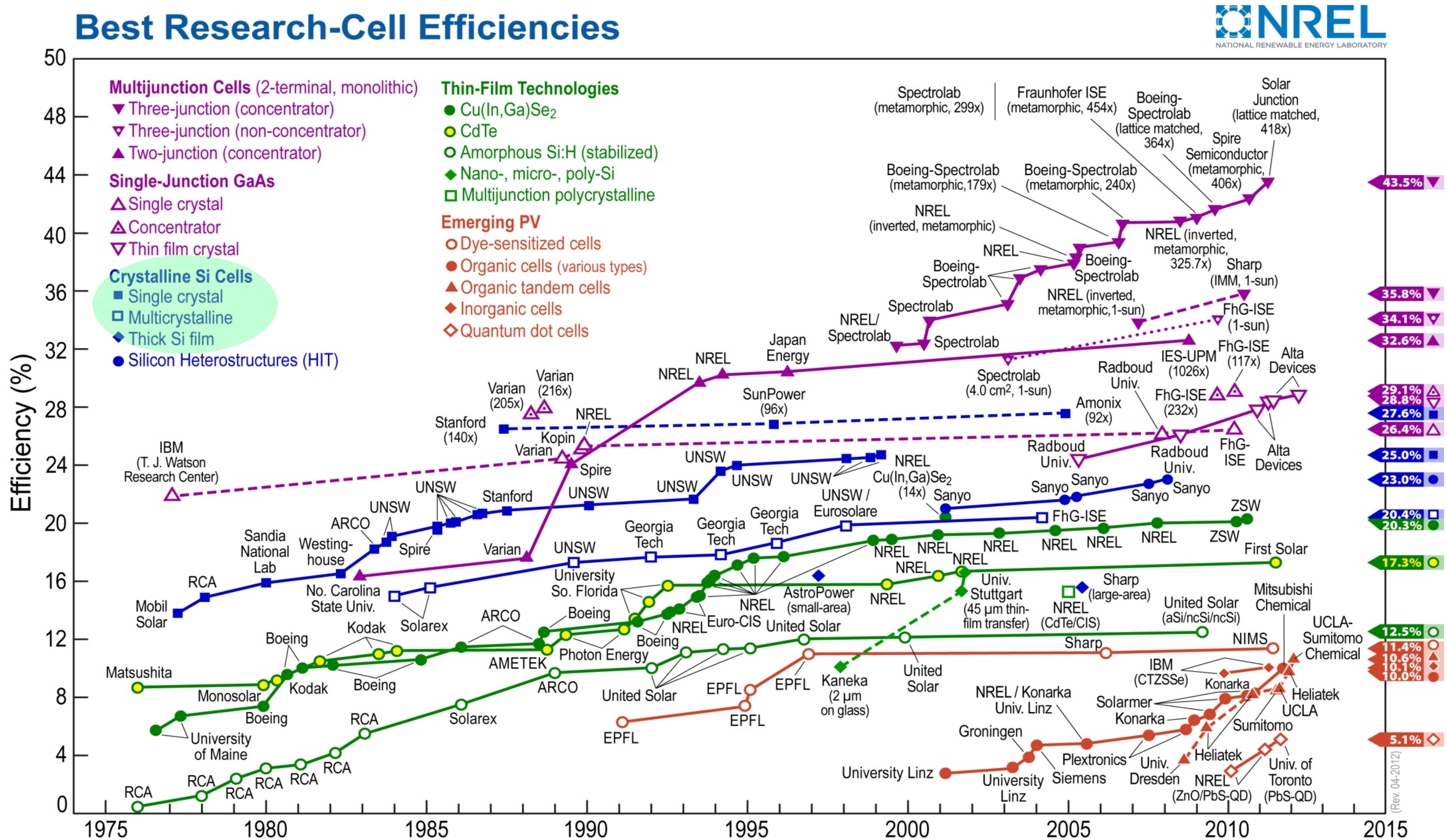
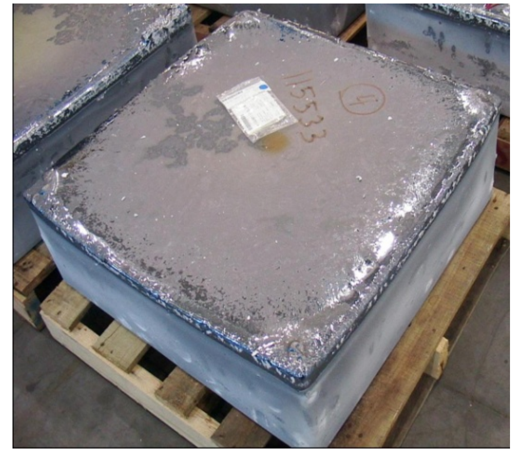


Example from NIST/NREL Website

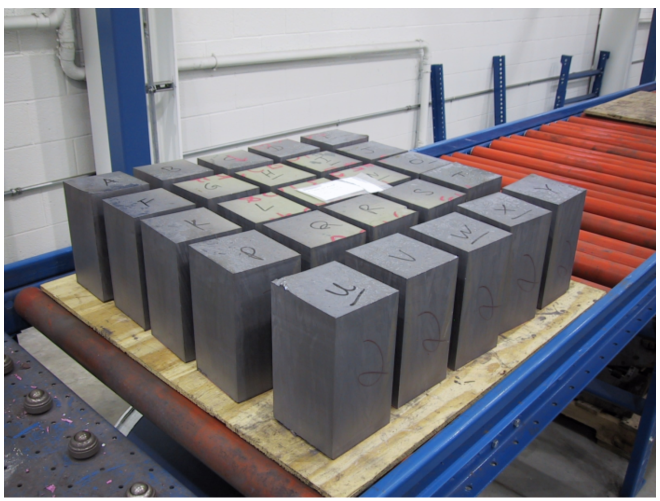
Multi-crystalline Ingot Solidification Process

Silicon “nuggets” - poly

Directional Solidification process: silicon pieces (“poly”) are melted, then frozen, in a ceramic crucible to form an ingot which in turn is cut into smaller “bricks”. Often called “casting”



Silicon Cast Ingot



Multi “bricks”

Multi Wafer

Multi Cell

Multi: 156mm square

Some photos from J. Posbic, “From Silicon to PV Grid Parity” August 2013

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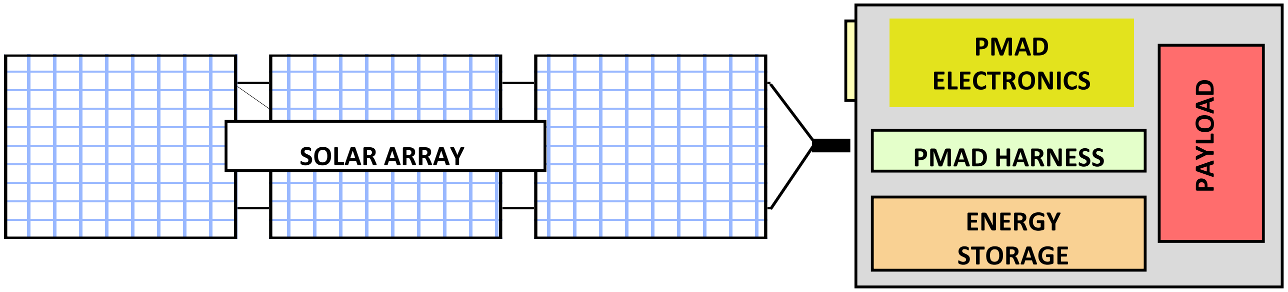
Why advance photovoltaic technology for space?

- **In present Earth-orbiting satellites ~ 20 - 35% of total mass and cost is the Electric Power System, the payload is ~ 23%**



↑ **Efficiency:** Drives area (A), mass (M), stowed volume (V), & cost

↓ **Size:** Drives launch vehicle, aerodynamic drag, radar cross-section, attitude control, & cost

↓ **Mass:** Drives payload fraction, launch vehicle, and cost

↑ **Lifetime:** Drives mission availability, mission lifetime, and life cycle cost

Chart from Dr. Sheila G. Bailey, NASA GRC, " The Future of Space Photovoltaics" (2013).

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Solar cell performance in space is different than performance underneath the atmosphere

Higher power (per unit area) above atmosphere

higher incident power:
Air mass zero = 1.37 kW/m^2
Air mass 1.5 = 1 kW/m^2

But

Lower efficiency

efficiency defined as power out/power in

Air mass zero efficiency typically ~85% of terrestrial efficiency

Chart from Dr. Sheila G. Bailey, NASA GRC, " The Future of Space Photovoltaics" (2013).

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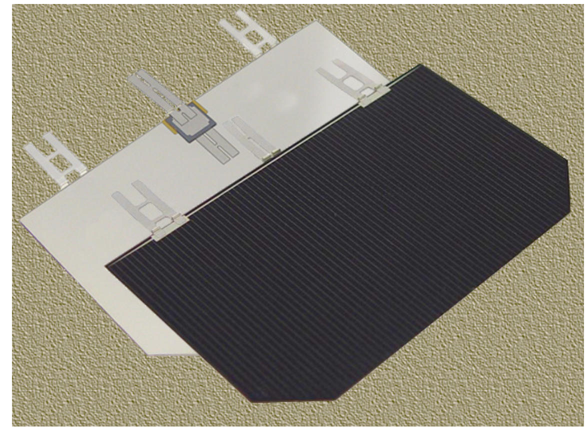
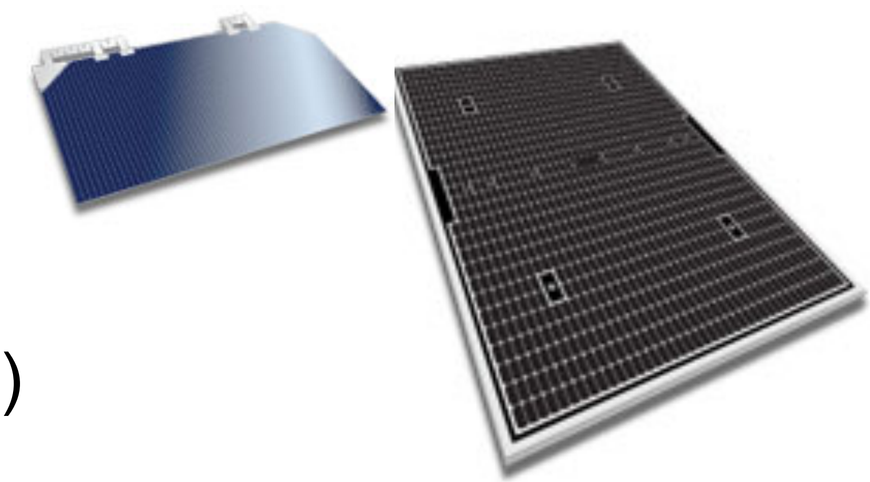
Higher Efficiency PV Approaches for Space

- Metamorphic Growth
- Inverted Metamorphic Growth
- 4, 5, … Junction Devices
- Dilute Nitride Devices
- Mechanical Stacking
- Optical Spectrum Splitting
- Concentrator Designs
- Quantum Confinement

(Quantum Wells, Wires, and Dots)



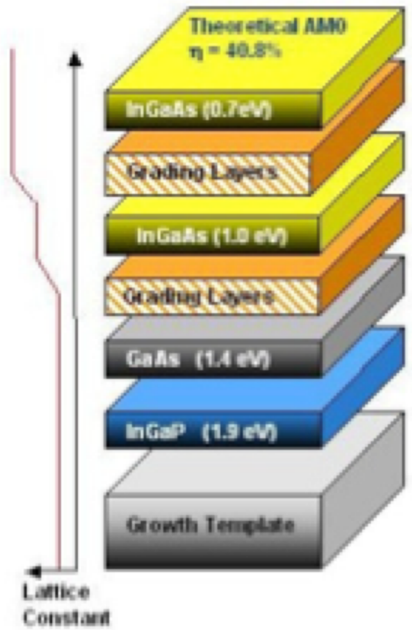


Efficiency from 30% to 40% and beyond?

Chart from Dr. Sheila G. Bailey, NASA GRC, " The Future of Space Photovoltaics" (2013).

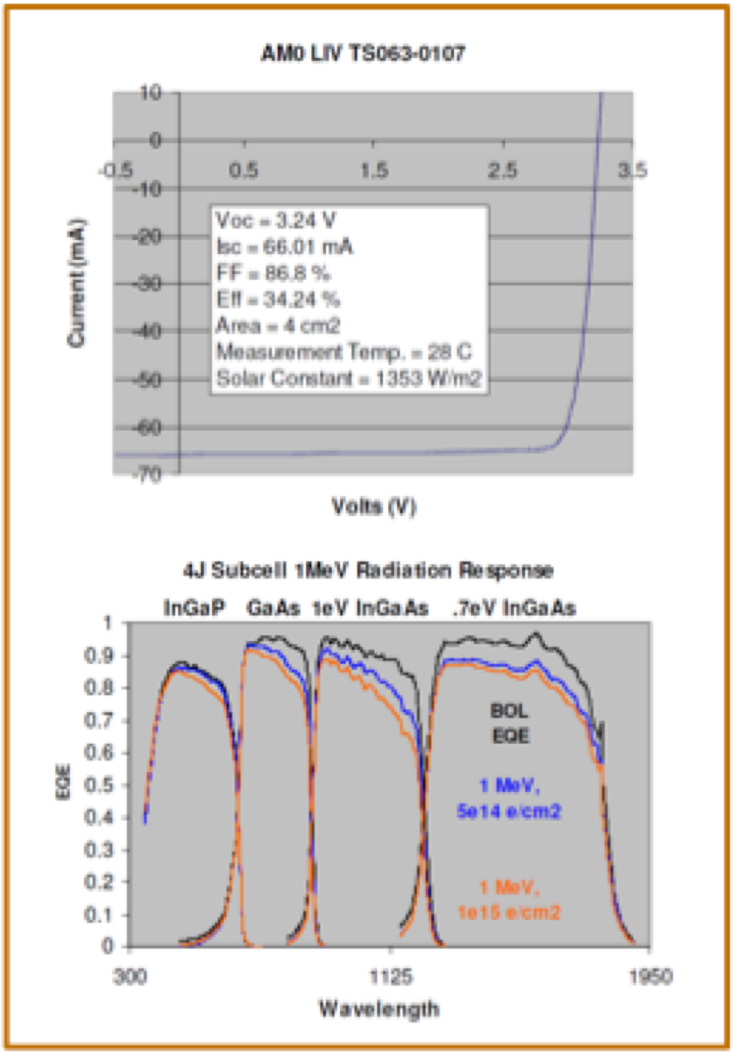
Inverted Metamorphic Multijunction (IMM) Development

IMM device concept preserves high performance top subcells while enabling current matched bottom subcells, resulting in a very high efficiency, very low mass solar cell.



P. Patel, 37th IEEE PVSC 2011

~ 36% AM0 Efficiency Demonstrated



4J IMM I-V performance and QE data after various radiation exposures

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