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

Materials in Space Workshop

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July 22, 2018

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

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Chart 1
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.
Directional Solidification Processes to Grow Single Phase Single Crystals

Czochralski (Cz) Process (Teal & Little)

Cz Crystals

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)
Segregation Studies (InSb)


Segregation Studies (Ge)

Segregation Studies (HgTe-CdTe)

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

Composition Maps $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$

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
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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Wafer is cut from crystal

Chips are made in Wafer

But...

Impurities distribution affects Chips (Segregation)

Impurities distribution both across and through wafer
1 D models of segregation

Axial Solute distributions during Solidification

- Melt Convection
- Complete mixing in Liquid
- No diffusion in Solid

Axial Solute distributions in Final Solid

- GS: $C_s = kC_0(1-g)^{k-1}$
- Complete mixing in Liquid
- No diffusion in Solid
- Gulliver-Scheil

BPS $k_{eff}$ does not predict initial/final transient; only $k < k_{eff} < 1$ (for $k < 1$)

BPS modification to GS: $C_s = k_{eff}C_0(1-g)^{k_{eff}-1}$

No Melt Convection

- No mixing in Liquid
- Thick Boundary Layer

Initial Transient

No diffusion in Solid

Initial Transient

No mixing in Liquid

After Fig 5.12, Chalmers
Ternary III-V Crystals

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

Problems from varying Composition / Lattice Parameter along crystal length
- Stress
- Cracking
- Cellular Interface leading to Polycrystal
- Twinning
- Electrical Characteristics
- Fabrication/Polishing
- Growth Process


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

Standard “Mono” Characteristics
- P-type
- Pulled by Cz technique
- Resistivity ~ 0.5-3 ohm-cm
- Nominal thickness ~ 160-190um
- Oxygen < ~ 10-18ppma
- Carbon < ~ 1 ppma
- 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
- AI BSF Cell Efficiency ~ 19.5+%; PERC ~ 20+%  

Standard “Multi” Characteristics
- P-type
- Directionally Solidified by Gradient Freeze technique
- Resistivity ~ 0.5-3 ohm-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
- AI BSF 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
“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?
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)
Potential Crystal Growth Processes to more fully exploit the Microgravity Environment


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
400mm-450mm Diameter Silicon


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

LOCOS isolation failure

Device leakage failures

Deep trench leakage

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

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


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

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Resistivity in Cz Silicon Crystal

Resistivity range effect on Yield: Boron dopant

Customer specification of resistivity range can greatly affect crystal yield and cost
Multi-crystalline Ingot Solidification Process

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”.

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).*
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/m²
Air mass 1.5 = 1 kW/m²

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).
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