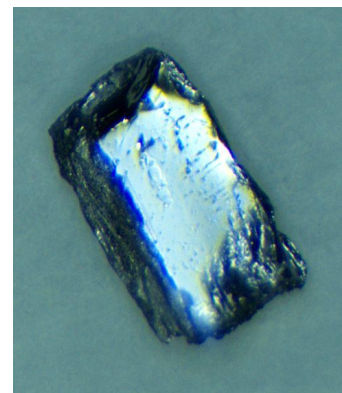


Synthesis and Characterization of BiTeI Single Crystals Using the Bridgman Growth Method

APS Far West 2025

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What is BiTeI?

BiTeI is a bismuth tellurohalide compound (BiTeX where $X = \text{Cl, Br, I}$)

- Semiconductor with reported band gap of 0.3-0.7 eV [1]
- Polar material (collection of different atoms within the unit cell makes it polarizable)
- Known in literature for strong spin-orbit coupling and noncentrosymmetric crystal structure
 - Rashba effect
- Possible applications in photovoltaics, spintronics, photodetection

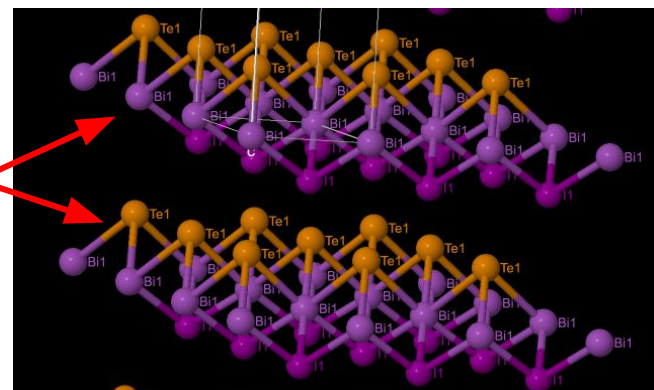
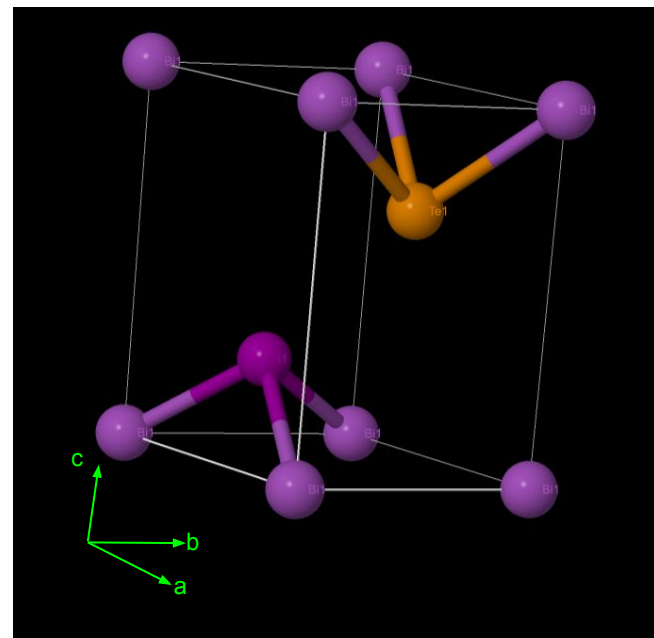
Crystal Structure of BiTeI

Trigonal space group $P3m1$

Lattice parameters ($a=4.3392\text{\AA}$ $b=4.3392\text{\AA}$ $c=6.854\text{\AA}$) [2]

- Crystallize in Hexagonal structure/Unit Cell
- Alternating layers of Bi, Te, and I along the c-axis
- Interlayer van der Waals bonding of tri-layer blocks allows exfoliation

Tri-layer Blocks



*Figures of structure pulled from ICSD database with reference [2]

Growing BiTeI

- Problem with growing BiTeI is the difficulty creating large single crystals and Bulk crystals
- Has been attempted with varying success
- Differing outcomes depending on growth method
 - Comparisons of growth techniques and difficulties forming single crystals explored in [3] and [4].

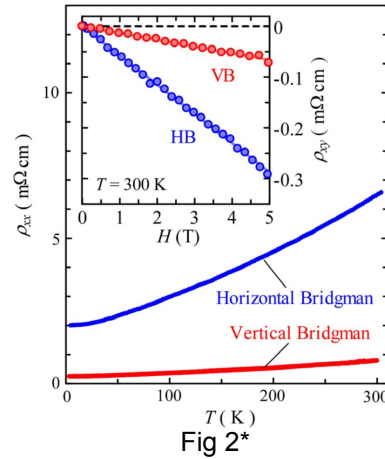


Fig 2*

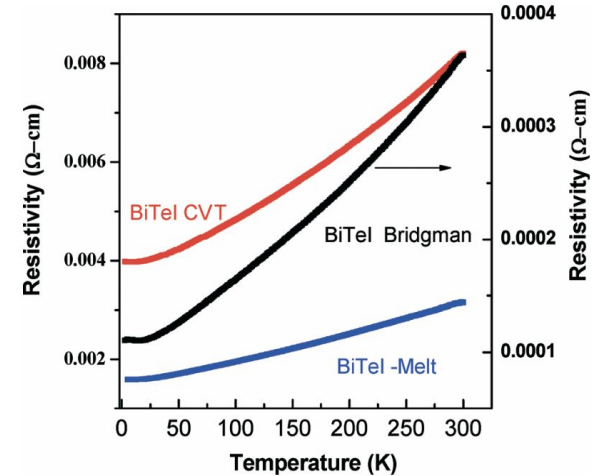


Fig 3*

* Figures 2 and 3 taken from references [3] and [4] respectively, placed here to showcase the difference in resistivity measurements.

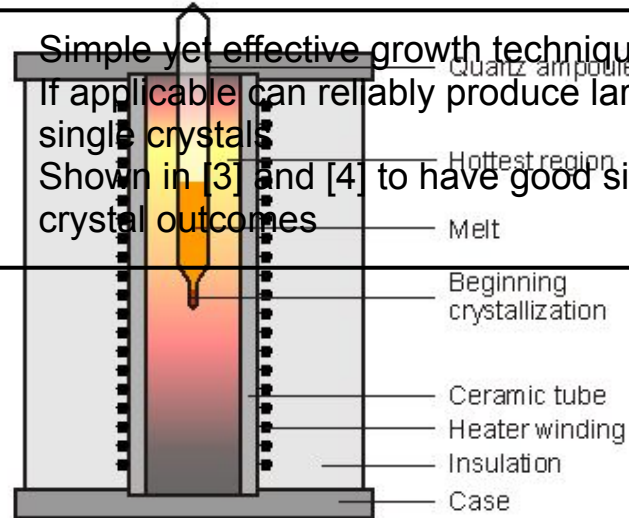
Bridgman Growth Basics

Bridgman Furnace

(Cross section)

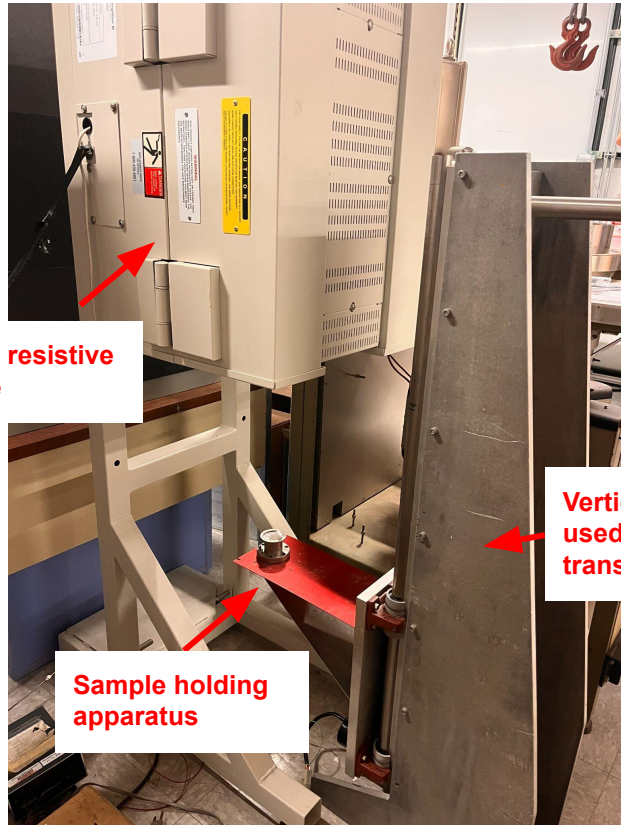
Why Bridgman?

- Simple yet effective growth technique
- If applicable can reliably produce large single crystals
- Shown in [3] and [4] to have good single crystal outcomes

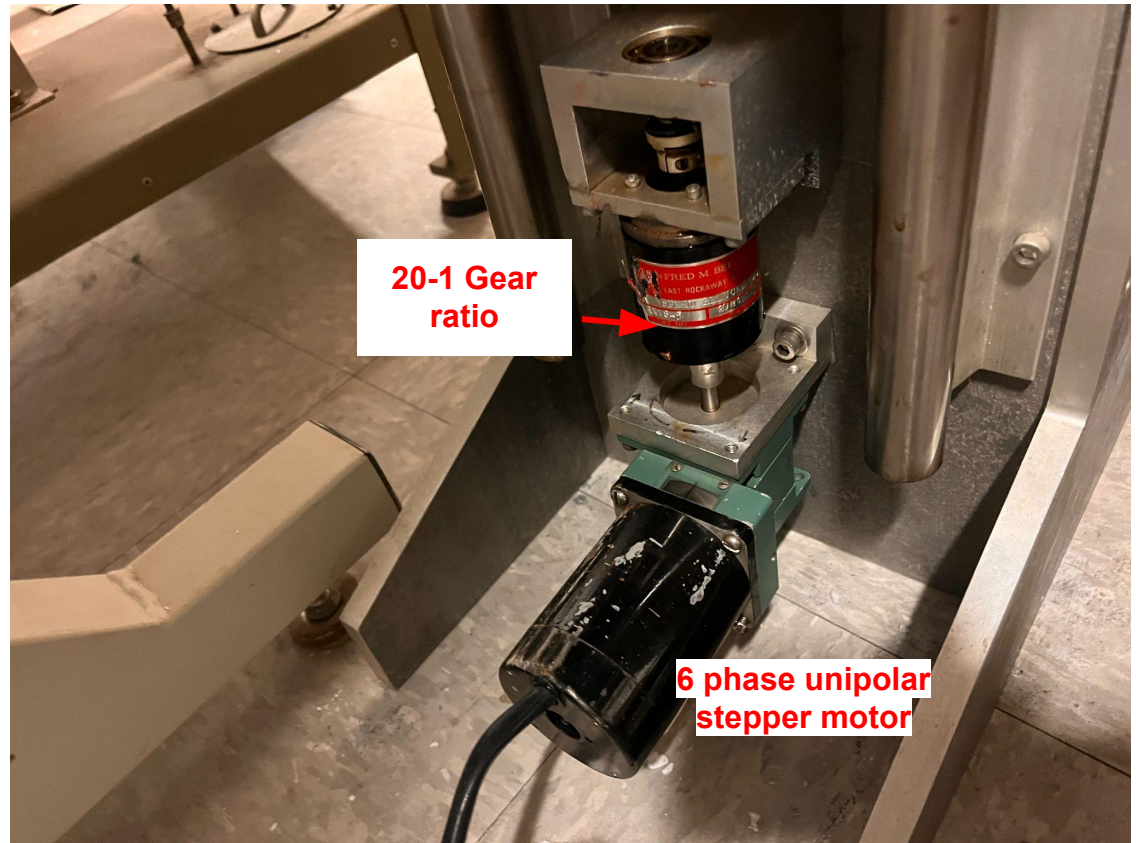
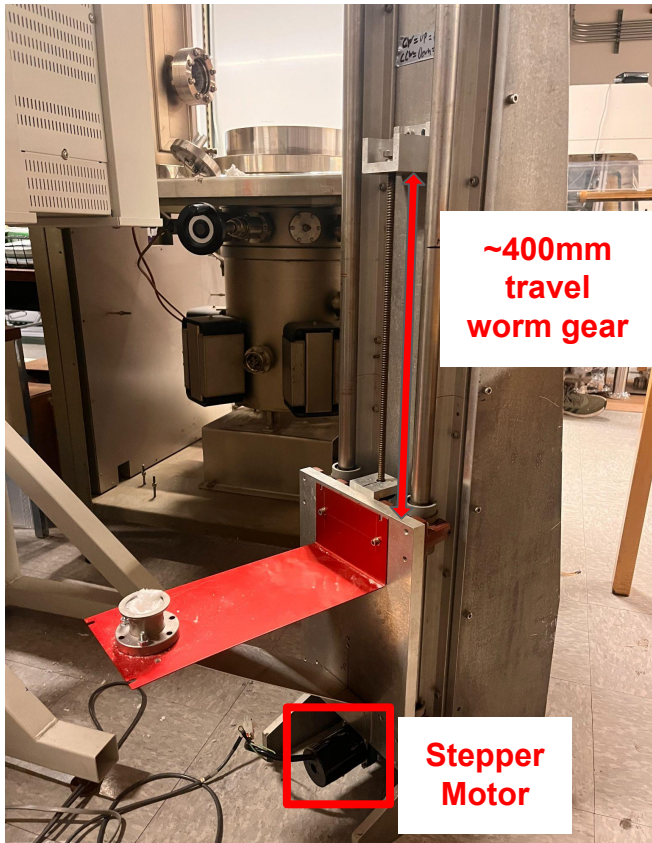


Animation pulled from [5]

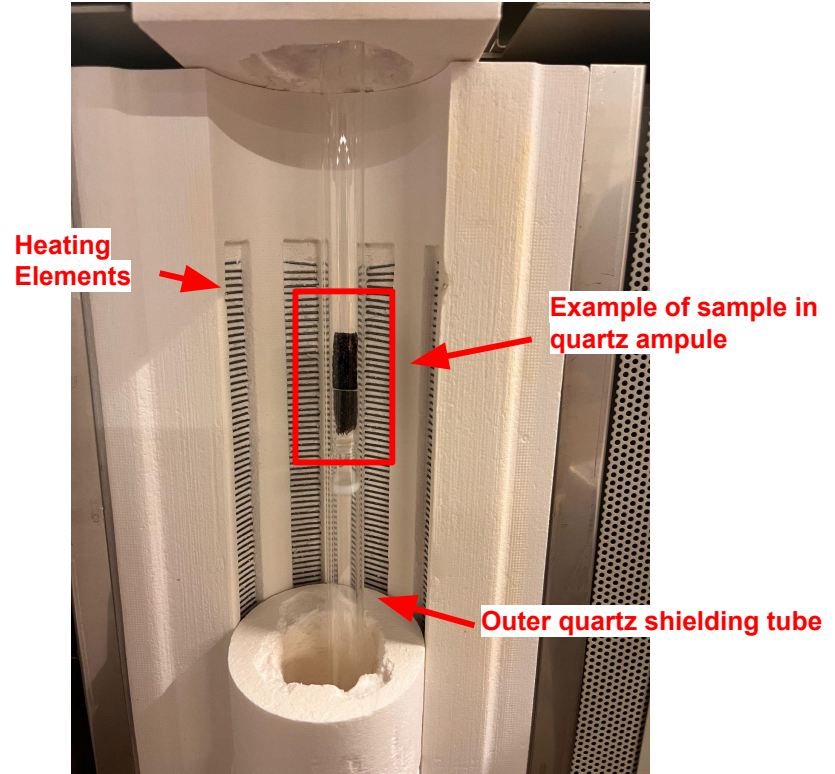
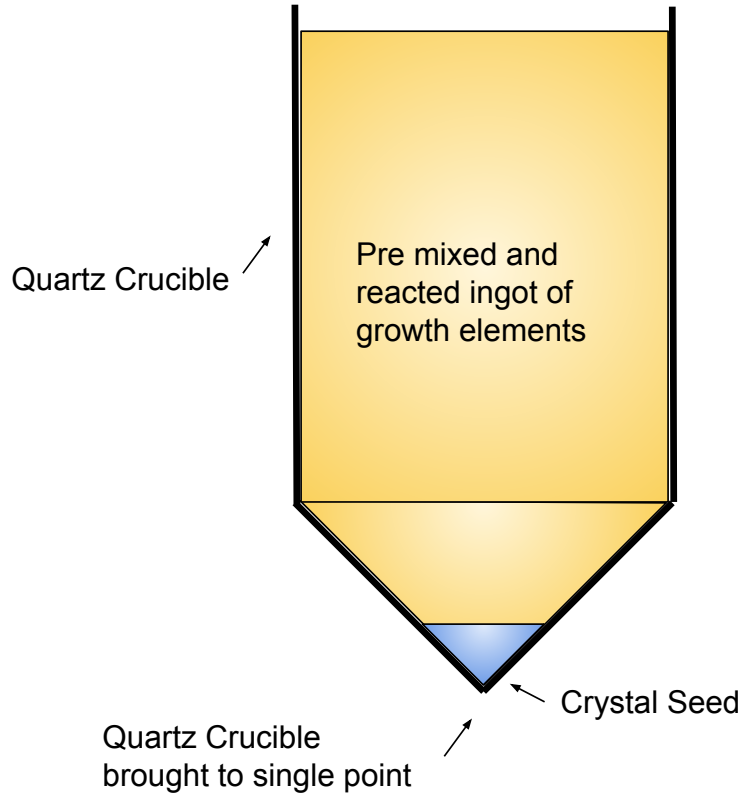
Our Bridgman set-up



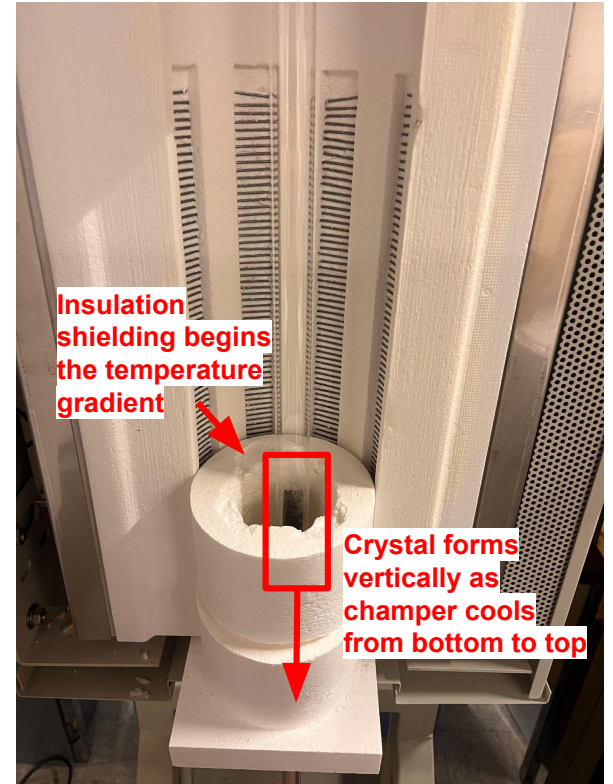
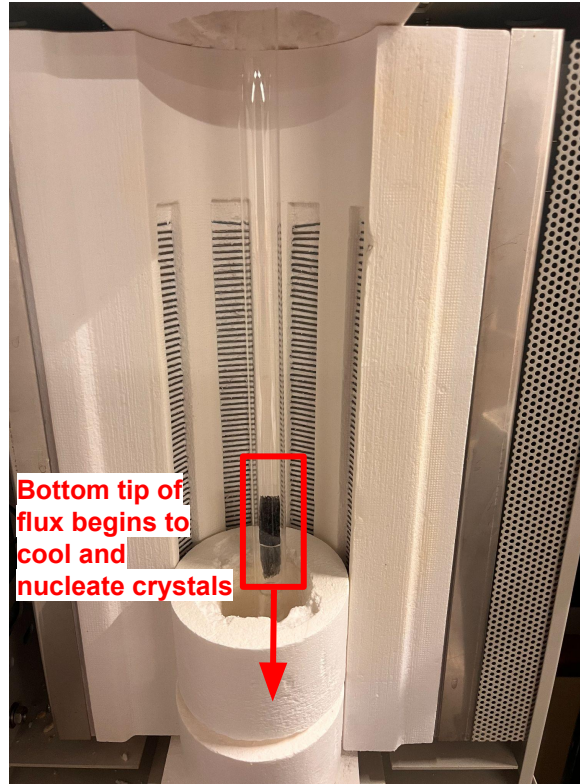
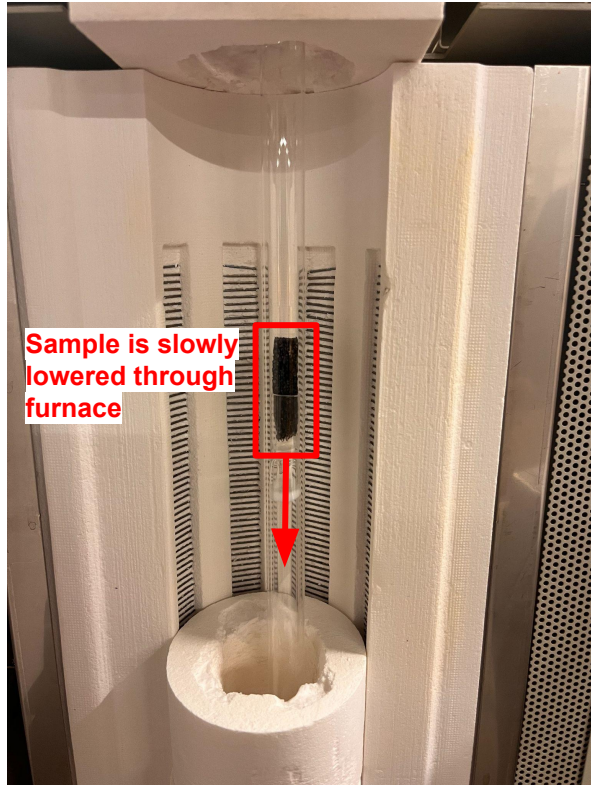
Unslide and Stepper Motor



Loaded Sample and Crucible Diagram



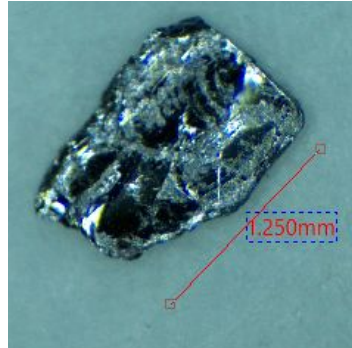
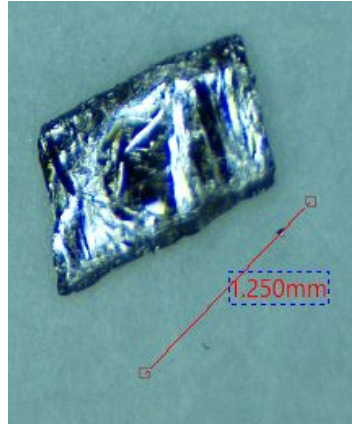
Sample Chamber



Our Growth Method and Results of Samples

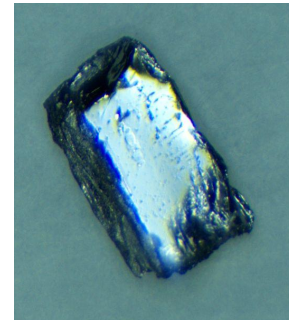
- Stoichiometric ratios of 1-1-1
- Elements Pre-reacted in a static resistive furnace to 500C to ensure proper mixing
- Vertical furnace temperature set to 500 C
 - Samples pulled through temp gradient of 500-400/350C before cooling to room temperature
- Used two growth timescales:
 - Two day pulled at rate of ~7mm/hr
 - Two week pulled at rate of ~20mm/day or 0.9mm/hr

Two Week



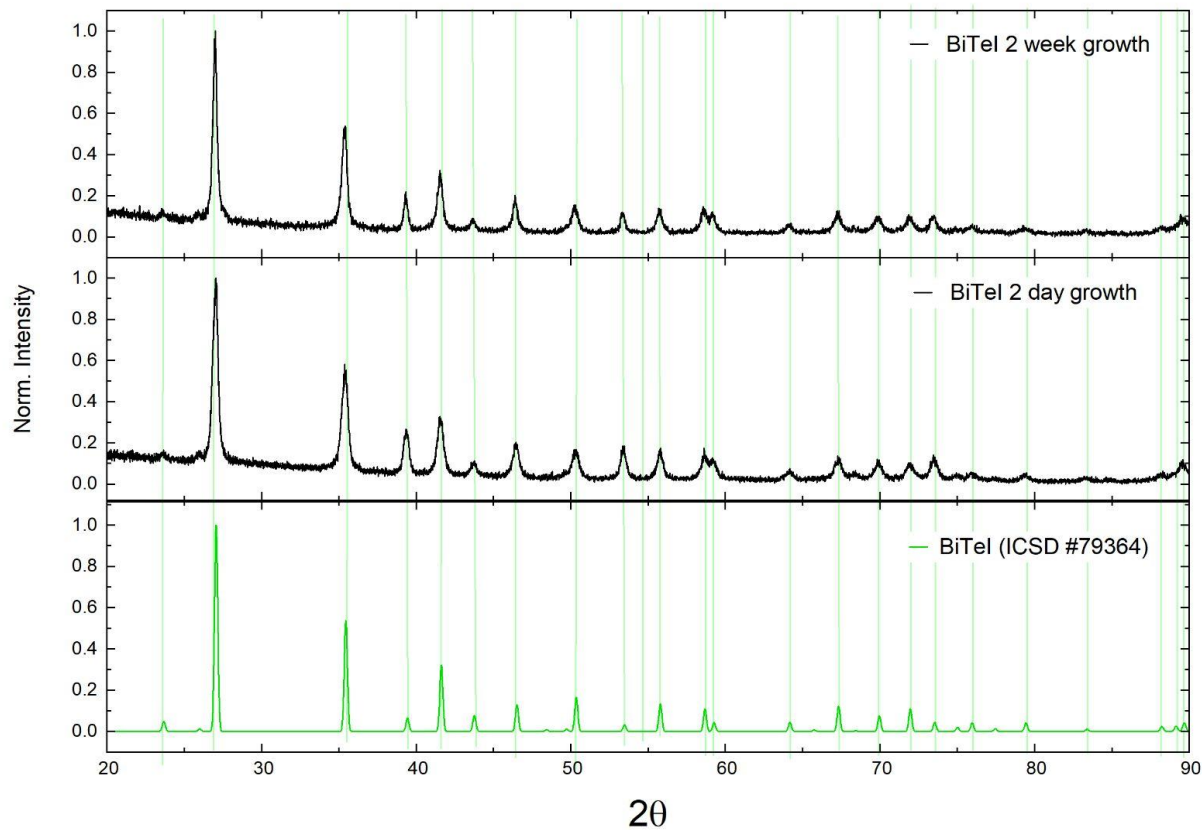
- Resulted in large single crystals
- Easily exfoliated along c-axis
- Grew with c-axis perpendicular to pull direction

Two Day

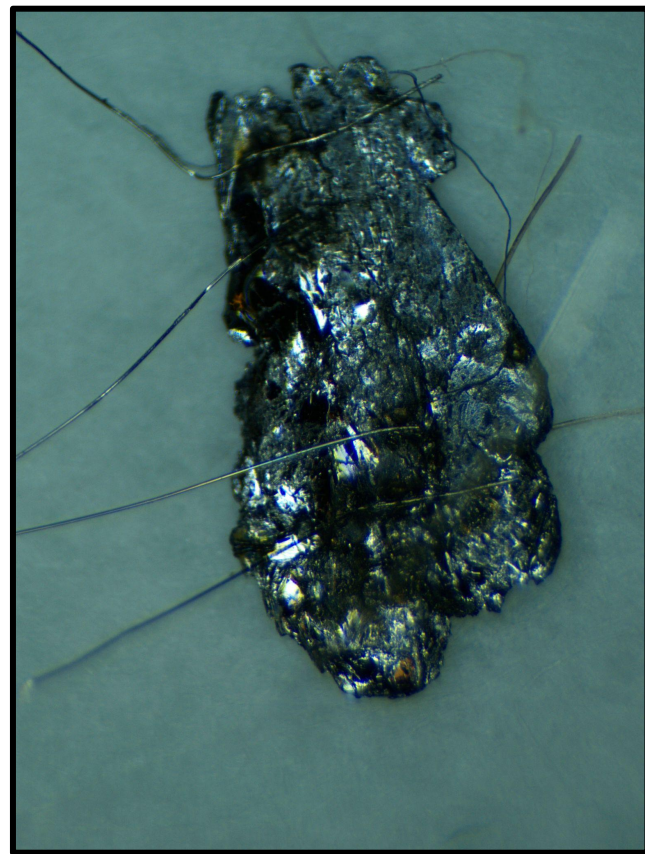
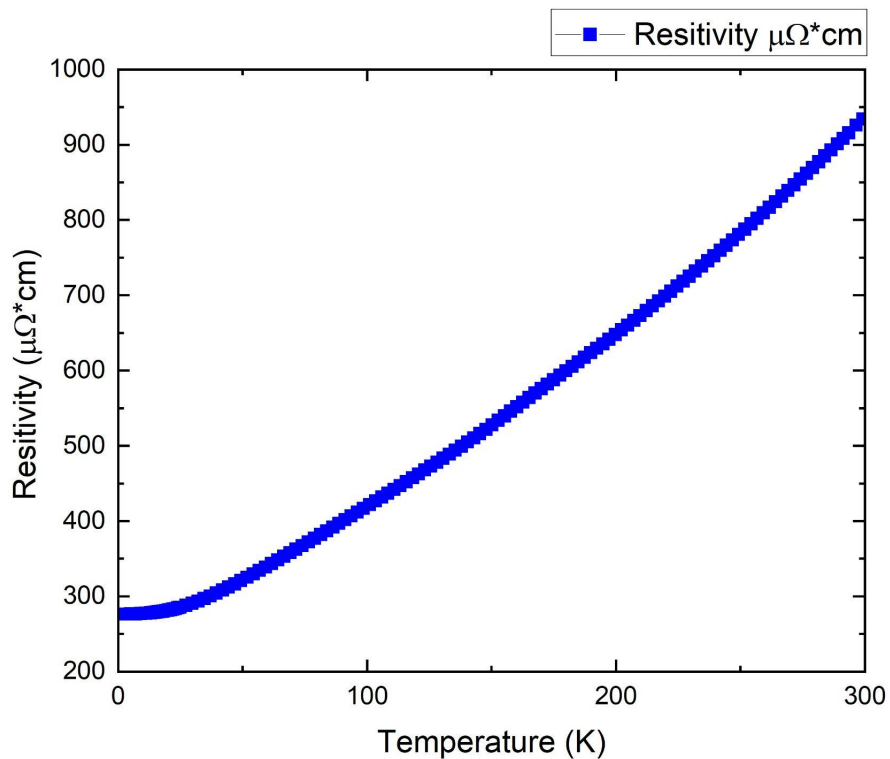


Growth Powder XRD Analysis

- Measurement with Rigaku MiniFlex (X-ray source-CuK α)
- Nice correlation between two week and two day growth
- Consistent with ICSD Data [2]
- Fairly confident we grew the intended phase of BiTeI

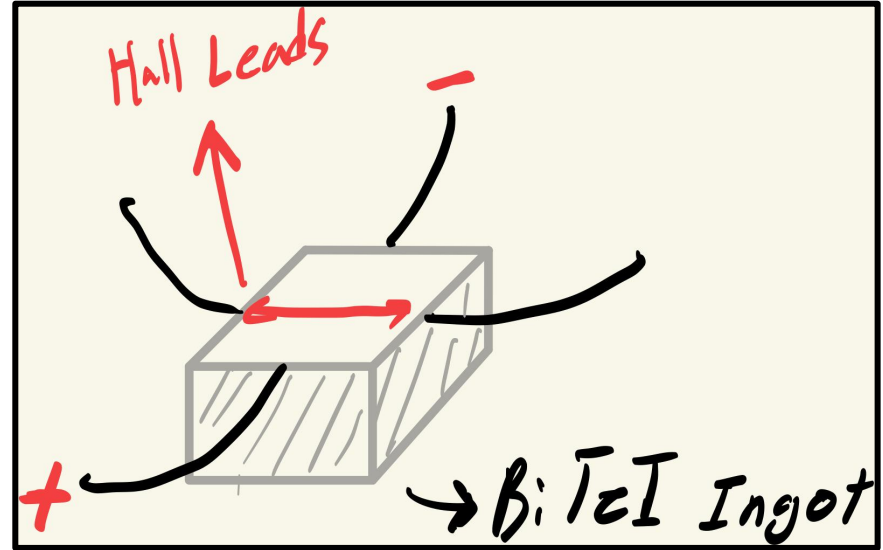


Two Week Growth Electric Transport (4 Wire Method)



Next steps

- We are able to grow large single crystals of BiTeI
- Iodine concentration is unknown
- We want to measure carrier density using Hall effect measurements which can help us understand iodine concentration
- Use intercalation or doping to induce complex magnetization or superconducting states



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Acknowledgements

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