SbSI Microrods as a Ferroelectric Solar Cell Absorber Material

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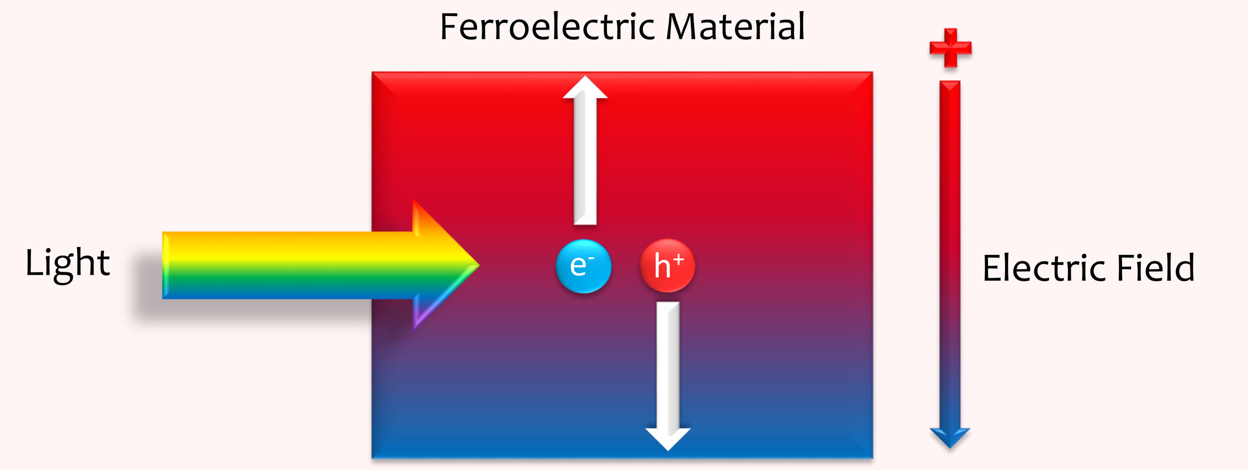
Background / Motivation

Solar photovoltaic energy is a clean and renewable source of electricity that has been researched heavily over the past 30 years. However, cost, toxicity, and rarity of precursor elements still limit widespread implementation of current technologies. Solution processing techniques, such as hydrothermal synthesis, are desirable due to their low cost and scalability. Yet, these methods generally produce materials of lower electronic quality with defects and impurities that can limit carrier collection. Ferroelectrics may be able to mitigate such drawbacks because of an internal electric field that can effectively separate carriers to reduce recombination rates, as shown in the schematic below. Antimony Sulfoiodide (SbSI) is a relatively unstudied ferroelectric with promising properties for solar cell absorber applications.



Synthesis Procedure

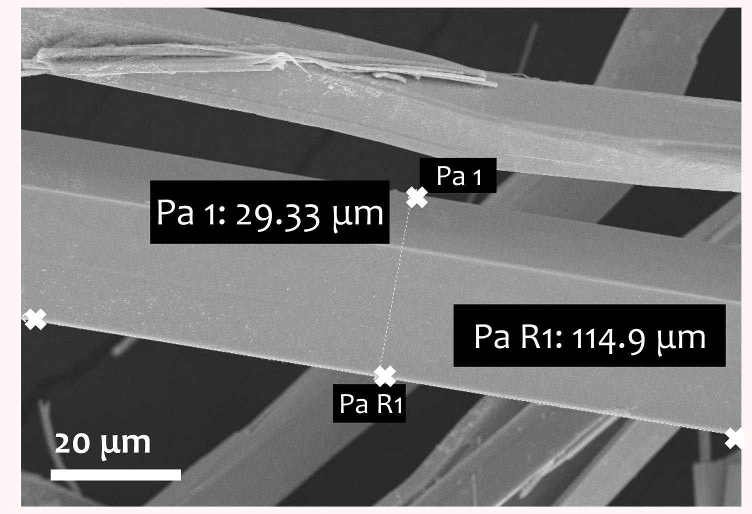
- Based on reported synthesis by Chen et al.
  - NH_4I, Thiourea, $SbCl_3$, and HCl added to Teflon-lined stainless steel autoclave (pictured on left)
  - Autoclave kept at 160° C for 4 hours
- After synthesis, crystals were washed with DI water and ethanol 5 times

Variances in pH and Seeding

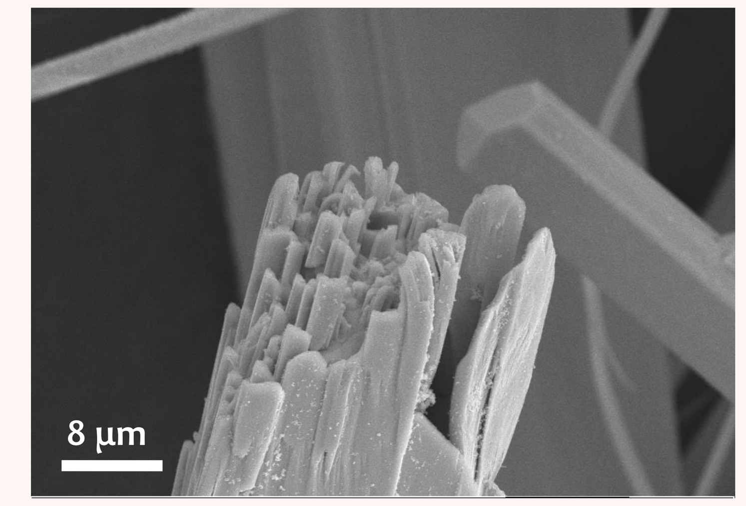
	1.0 M HCl Crystals	1.8 M HCl Crystals	Nucleated Seed Crystals
Precursor Elements	NH_4I, Thiourea, $SbCl_3$	NH_4I, Thiourea, $SbCl_3$	NH_4I, Thiourea, $SbCl_3$, 1.8 M HCl Crystals
Reaction Temperature	160° C	160° C	140° C
Concentration of HCl Used	1.0 M	1.8 M	1.0 M
Precipitate Color	Dark Brown	Dark Red	Light Purple

Morphology

Dark Red 1.8 M HCl Crystals under Light Microscope

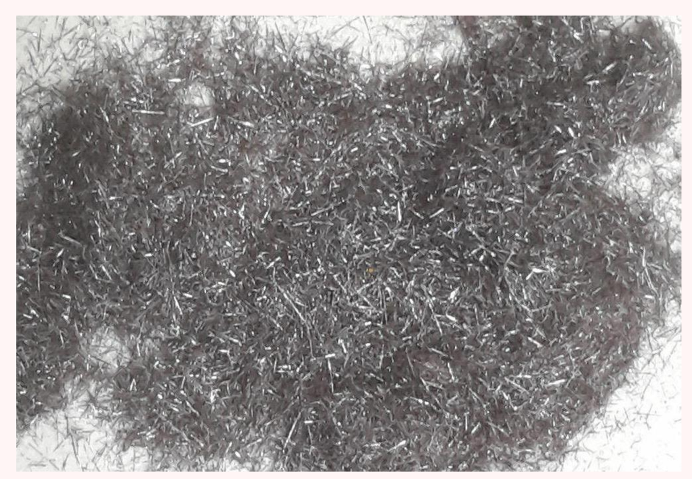


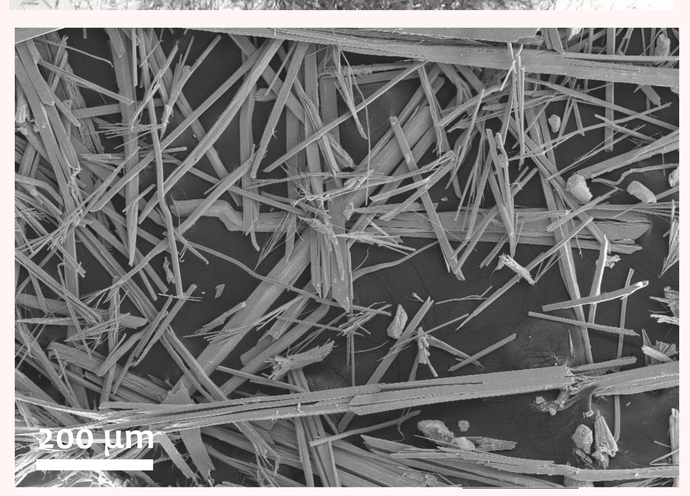
All crystals averaged 650 microns in length and 30 microns in diameter



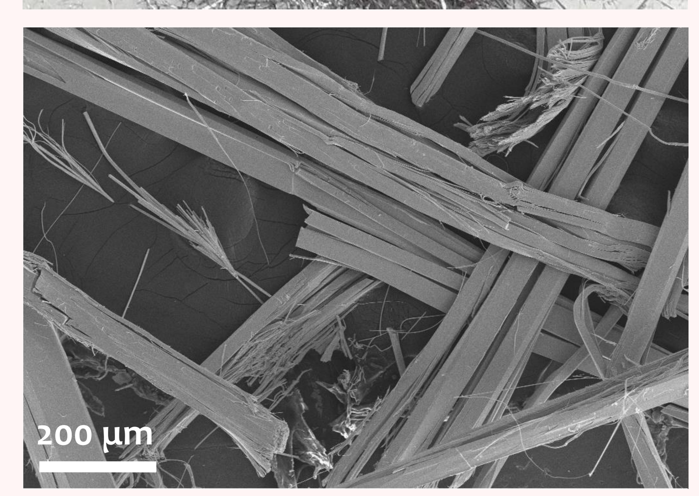
Evidence of Highly Crystalline Branching in 1.0 M HCl Crystals

Effects of pH and Seeding

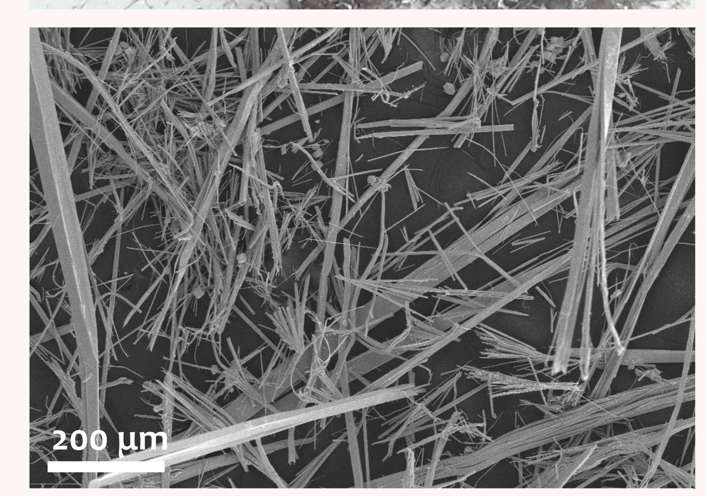




1.0 M HCl Crystals

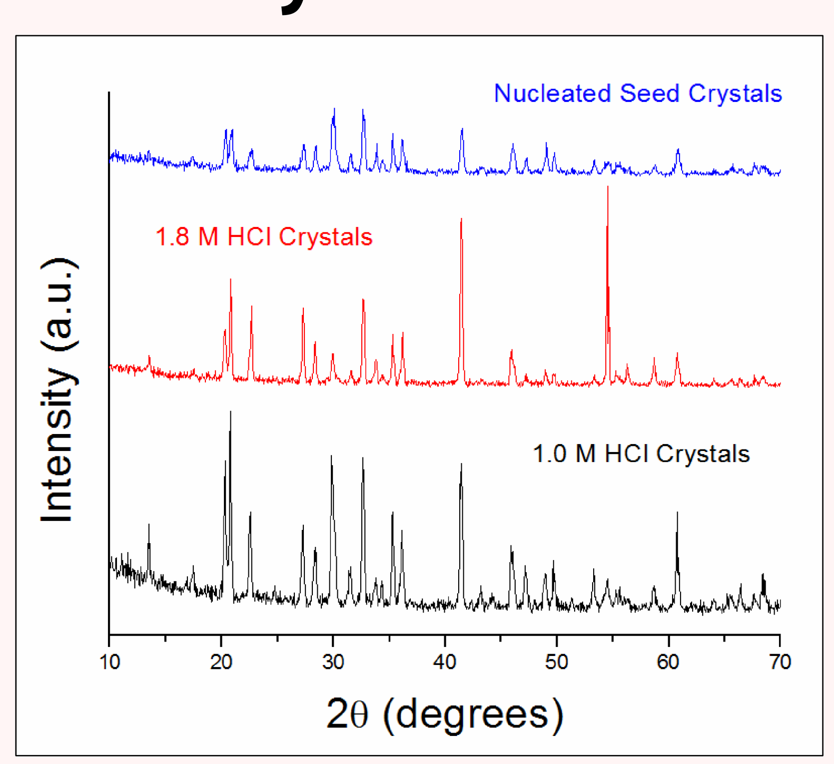


1.8 M HCl Crystals

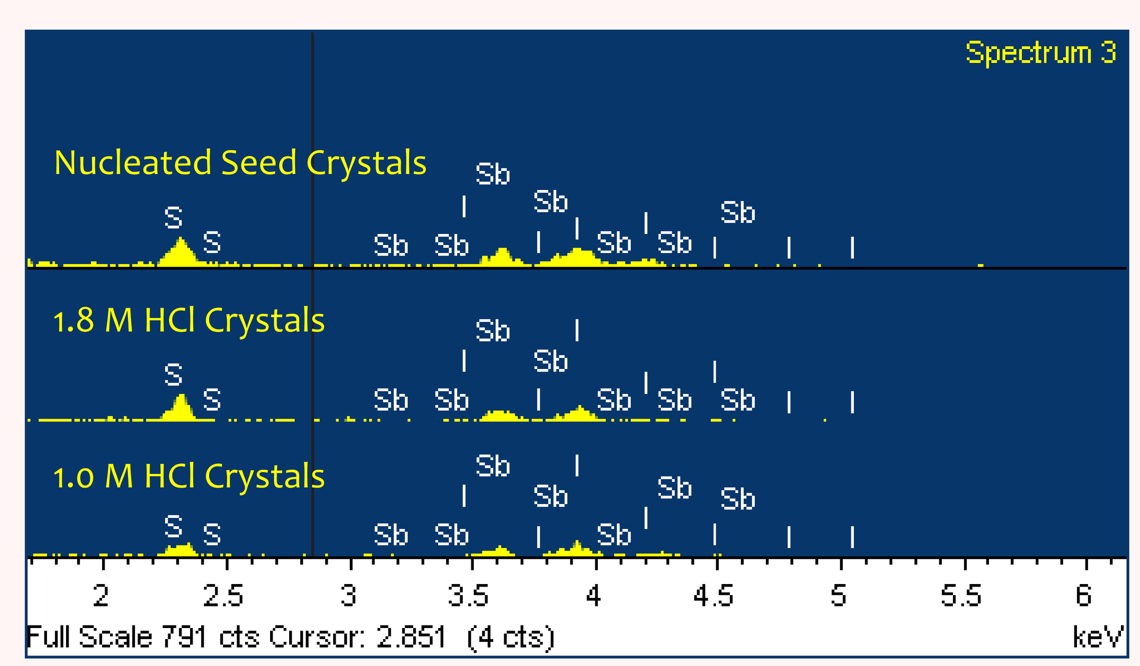


Nucleated Seed Crystals

Crystal Structure and Chemical Composition

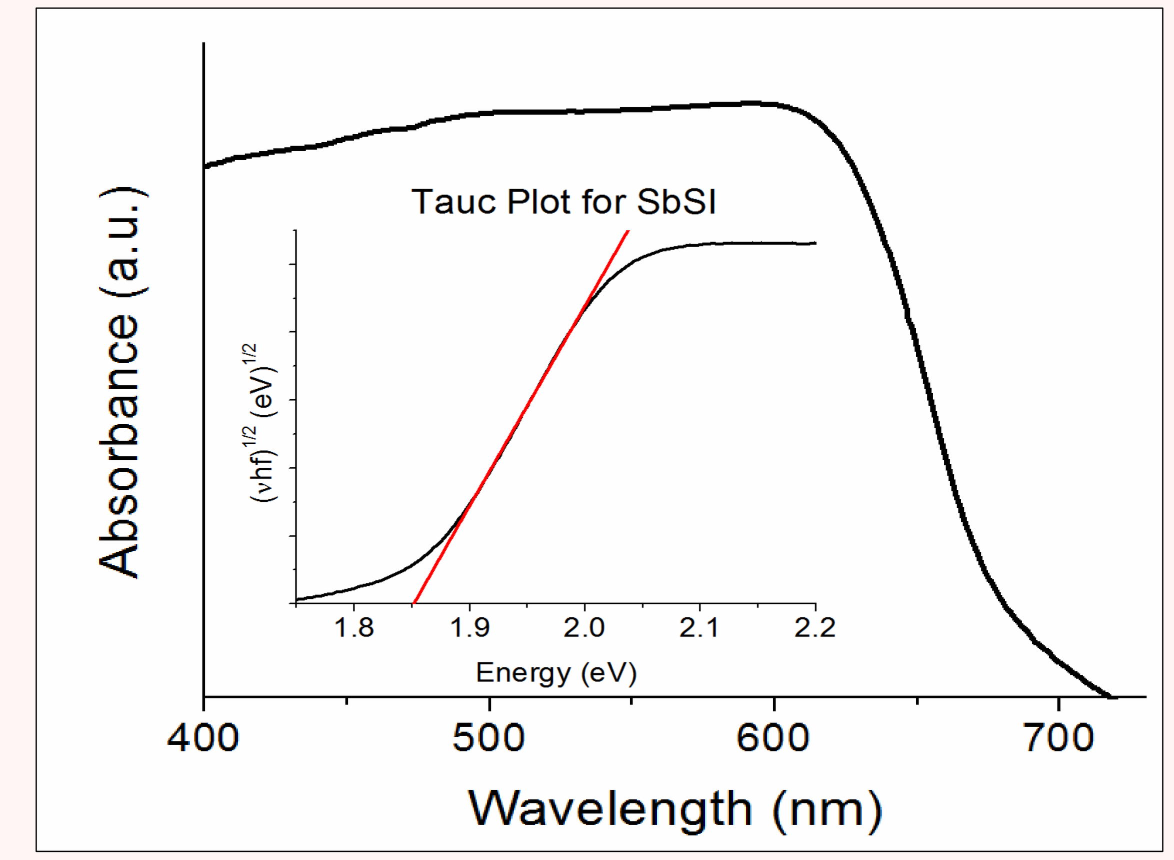


XRD analysis confirms crystal structures, but varied intensities suggest differences in crystal orientations from standard SbSI



EDS analysis confirms chemical composition of all reaction conditions

Optical Characterization



- Estimated indirect band gap of **1.85 eV** via the Kubelka-Munk equation: $f(R) = \frac{(1-R)^2}{2R}$
  - R : absolute reflectance of the sample layer
  - Indirect band gap E_g estimated by extrapolating linear portion of Tauc plot

Future Work

- Evaluate further pursuit of this promising absorber layer
  - Measure mobilities and carrier lifetimes of SbSI through ultrafast terahertz spectroscopy
  - Determine axis of polarity
  - Analyze internal electric field and its effect on carrier separation
- Nucleate larger crystals as seed crystals
- Characterize ferroelectric and piezoelectric properties of SbSI

Reference

Chen et al., *RSC Advances*, 19 Feb 2015. *DOI* : 10.1039/C5RA01180A

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