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Thermal diffusion behaviour of Li on surfaces of HOPG, Si(111) and SiC-6H measured with LEED and AES

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INTRODUCTION

- **GOAL:** To observe lithium reactivity and mobility on highly oriented pyrolytic graphite (HOPG), silicon (111), and silicon carbide (6H)
  - Samples are potential anode and cathode materials for lithium-ion batteries
- Use of Low Energy Electron Diffraction (LEED) and Auger Electron Spectroscopy (AES) for analysis

MOTIVATION

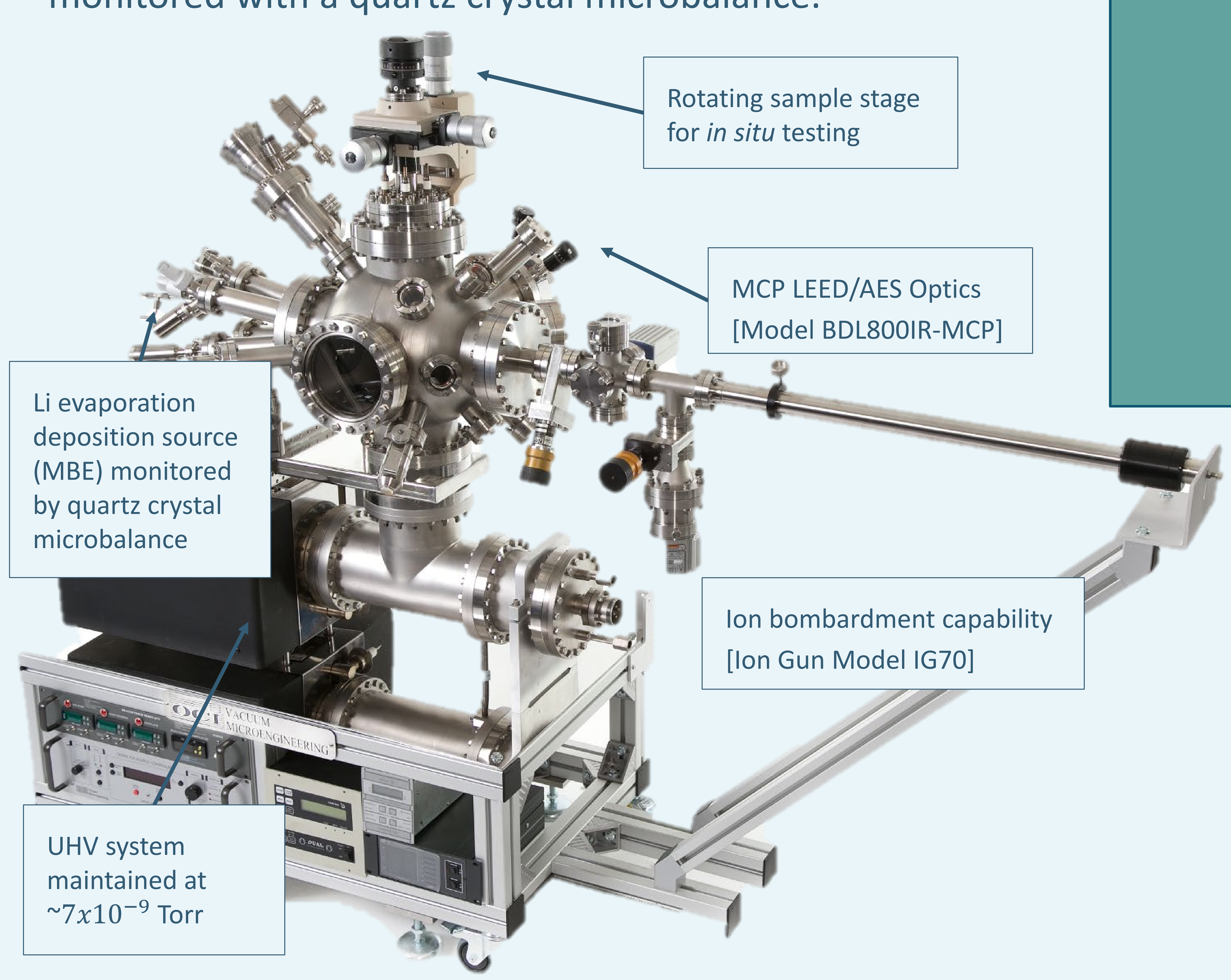
Most current battery development research is focused on the improvement of battery properties such as:

- Maximum capacity
- Power density
- Solid state electrolyte solutions
- Cycle life

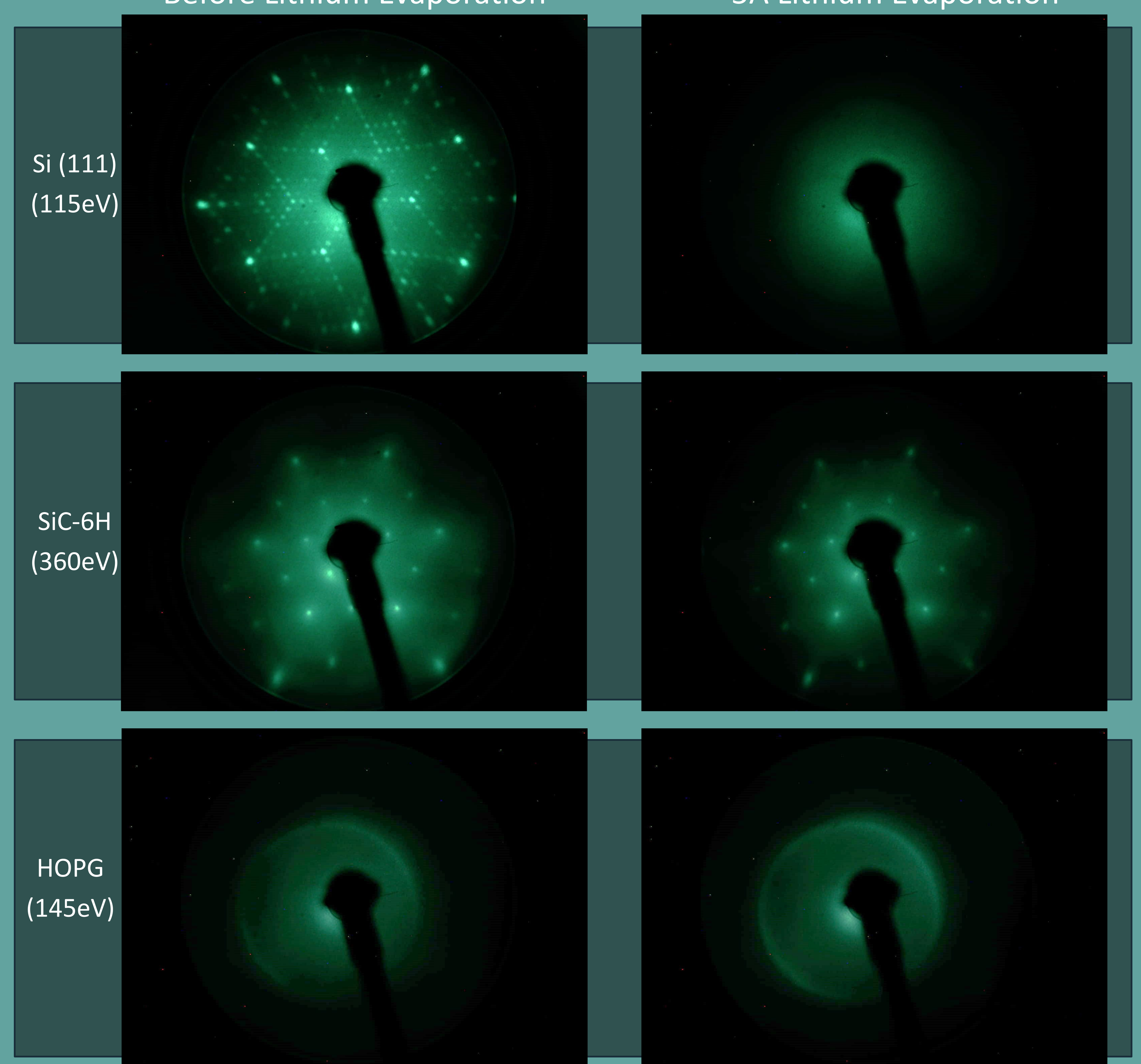
In this study, we direct our attention to fundamental aspects of the battery anode materials with respect to lithium diffusion. Deposition of Li on surfaces of relevant materials with structural characterization will demonstrate thermal Li behaviour, presenting possible links to Li diffusion mechanisms for novel battery designs.

EXPERIMENTAL SETUP

Testing was completed in an Ultra-High Vacuum (UHV) system utilizing Li evaporation and high-temperature annealing (Model IMBE300-SPH). Li evaporation was monitored with a quartz crystal microbalance.



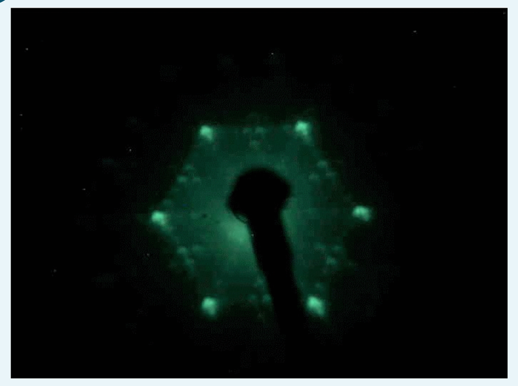
Significant room temperature **Li diffusion** on **HOPG** and **SiC-6H** associated with unchanged surface **crystallography**



No room temperature **Li diffusion** on **Si(111)** observed in drastic surface **crystallography** change

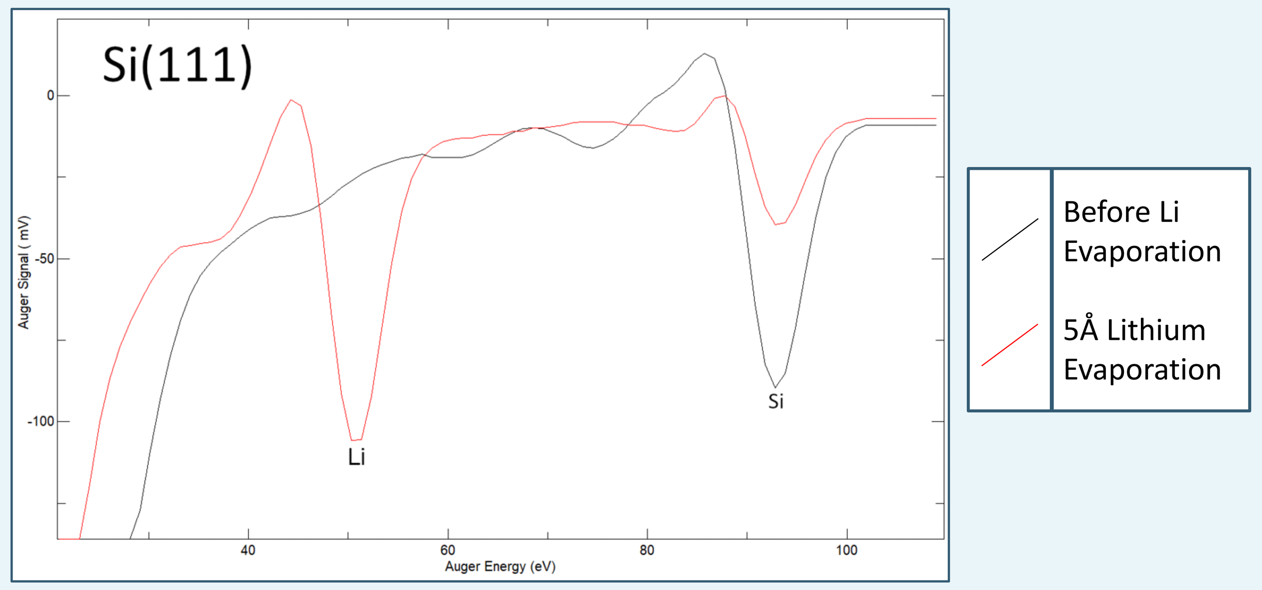
PROCEDURE AND RESULTS

1. Good surface crystallography obtained

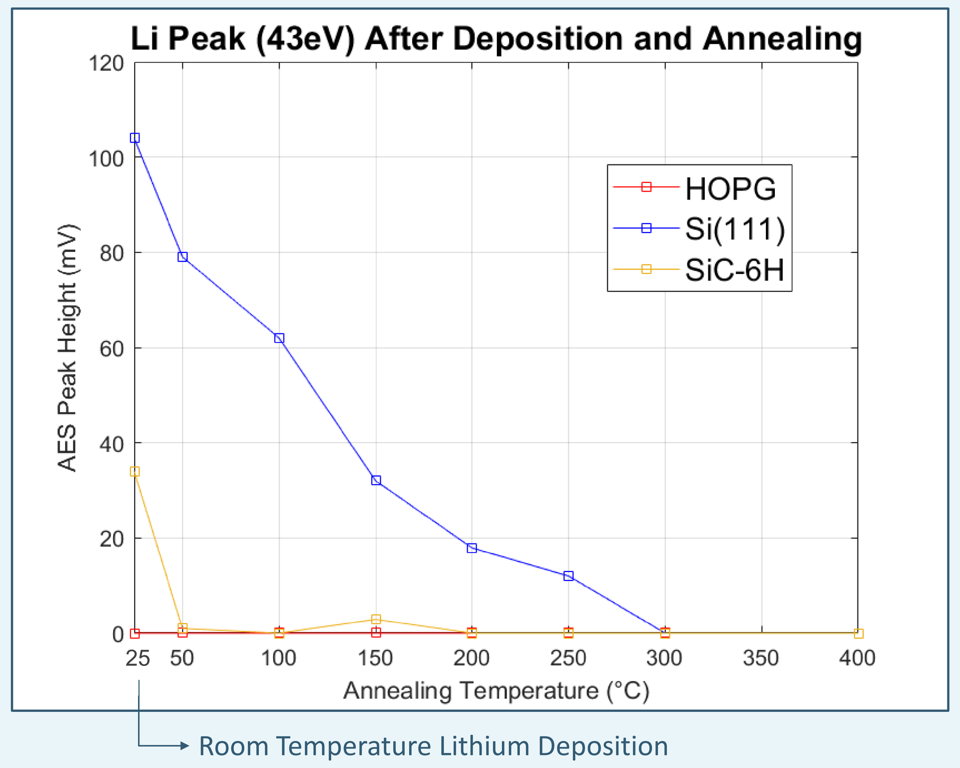


- Si(111) annealed to 800°C
  - Shown here
- SiC-6H annealed to 950°C
- HOPG cleaved

2. 5Å of lithium evaporated



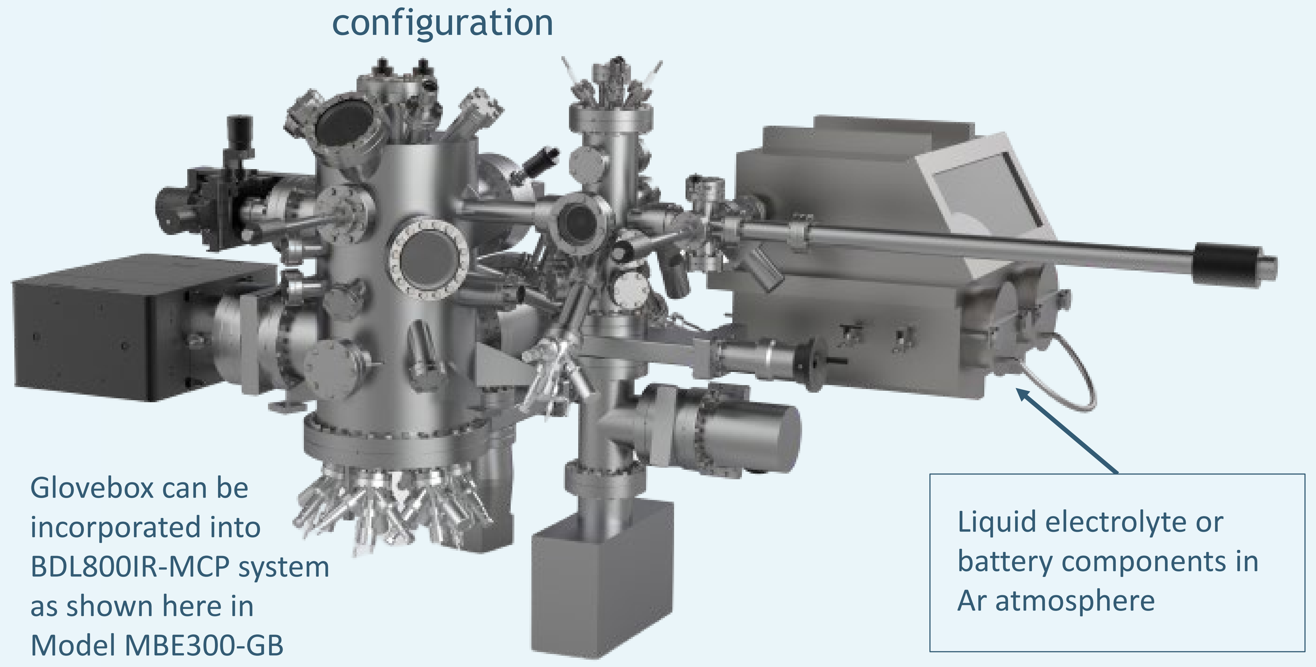
3. Annealed from 50°C to 800°C



- AES scans on plate confirm successful Li deposition on HOPG and SiC-6H
- Timed AES scans on SiC-6H reveal room temperature diffusion over the span of approximately 1 hour

FUTURE RESEARCH

- Probing anode and cathode materials with a liquid electrolyte
  - Following Li deposition and diffusion, the sample can be moved to the liquid electrolyte (in the glovebox) and moved back after interactions for further testing (LEED/AES characterization before and after electrolyte contact)
  - Full battery integration is also possible in this configuration



DISCUSSION

The reactivity of Si makes it a challenging anode material, despite high theoretical capacity

Results depicted a persistent AES Li peak during annealing and crystallography destruction immediately following evaporation (evident in LEED data)

Literature shows interstitial Li diffusion with interactions between native Si atoms and Li atoms. Interaction causes expansion and destroys surface crystallography (as shown in LEED data)

Silicon carbide displayed much greater stability when in contact with lithium, comparable to graphite (the dominant anode material)

The LEED surface crystallography data and AES data taken from the sample cover and sample plate on both samples confirms the diffusion of lithium at room temperature, without impairing surface crystallography

Literature shows interstitial Li diffusion as a mechanism in HOPG and SiC-6H; however, LEED and AES data suggests native atom interaction is not crystallography-altering

Future battery development could benefit from this methodology of using AES to observe thermal lithium diffusion tendencies for characterization of possible solid-state battery materials.