

A new method for evaluating Li-ion battery anode materials based on “natural” Lithium diffusion characterization



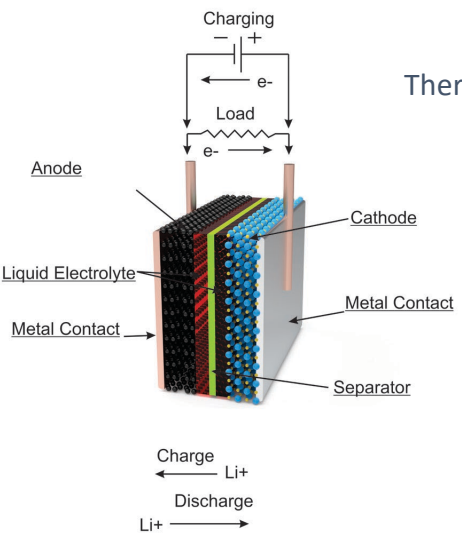
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Problem - key properties of electrode materials are not tested before battery cell assembly

Solution - characterization of “natural” Li thermal diffusion on battery electrode materials

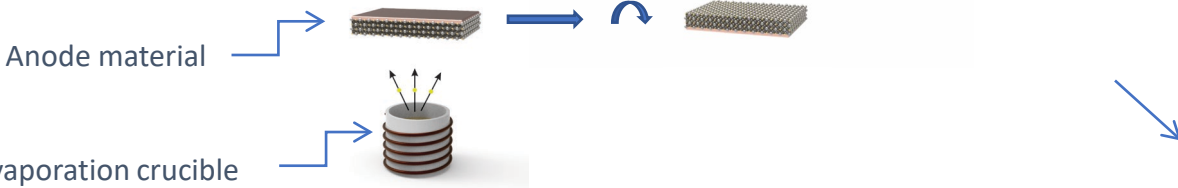
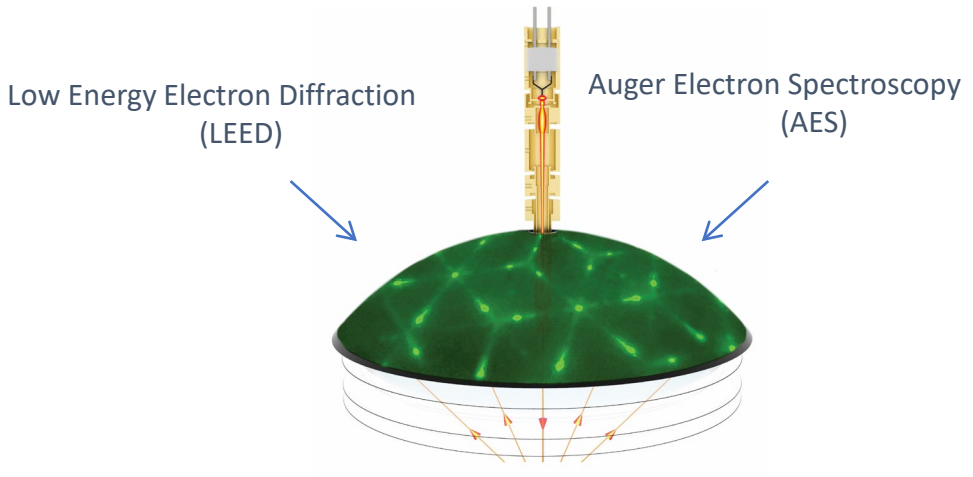
Li diffusion in electrode material - key factor for battery performance

Liquid Electrolyte Battery Cell



There is no Li diffusion tests on battery electrodes

Nanoscale materials problems (structural and compositional) is effecting:
 Lost battery capacity
 Reduced cycle life
 Dendrite growth



! Novel Methodology !

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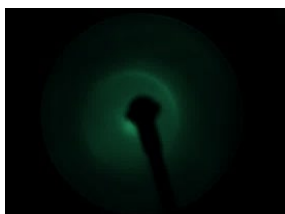


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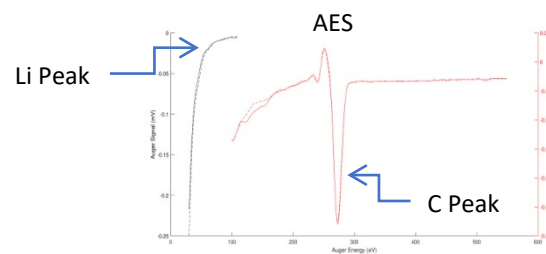
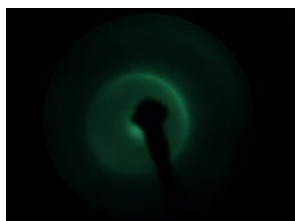
LEED and AES Data & Conclusions

HOPG (Graphite) – strong Li diffusion, no change to surface crystalline structure

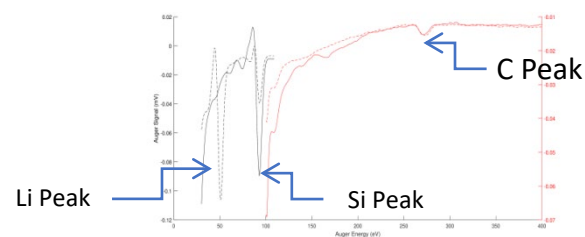
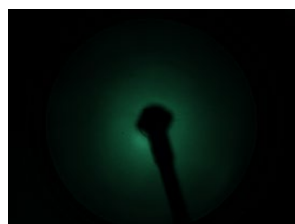
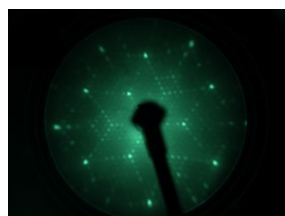
Before Lithium Evaporation



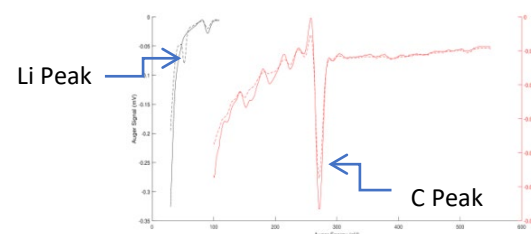
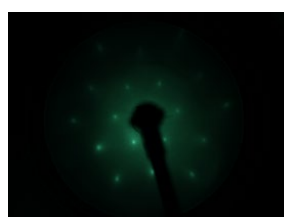
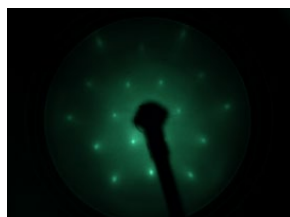
5Å Lithium Evaporation



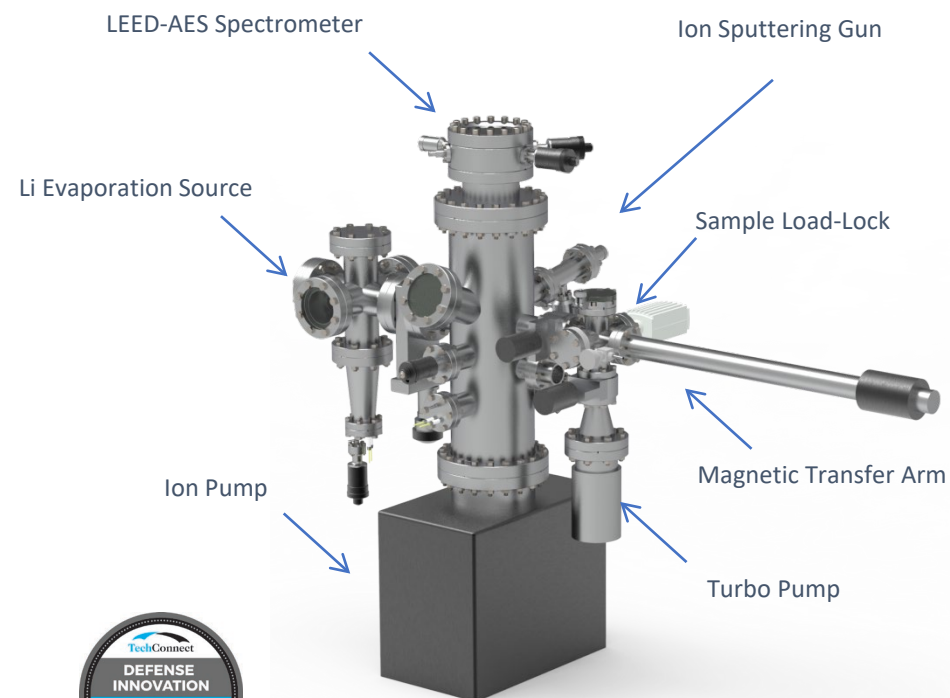
Si(111) – no Li diffusion, drastic change to surface crystalline structure



SiC-6H – some Li diffusion, small effect on surface crystalline structure



UHV System for Li thermal diffusion tests - early indicator of battery materials performance



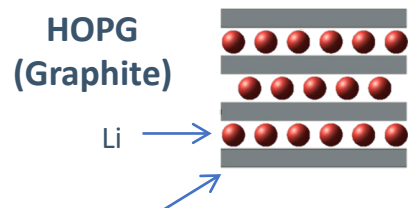
<https://events.techconnect.org/DTCFall/awards.html>

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Conclusions

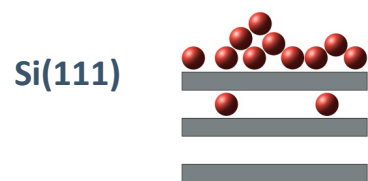
We identified 3 categories of the materials that can be used for the Li battery anode:



Structure of atomic layer

“Graphite - like” : Materials with “natural” rapid Li diffusion properties and no effect on structural order

Similar: LiNbO₃-Mg doped



“Silicon - like” : Materials with no “natural” Li diffusion and strong effect on structural order – polycrystallization or amorphization

Similar: Si(100), Si(211)

Silicon requires nano-engineering process to create the Li diffusion path



“Silicon carbide - like” : Materials that have good “natural” Li diffusion and low effect on structural order

Similar: Diamond CVD

- The most desired material for the high energy density:
 - Strong “natural” Li diffusion properties or intercalation
 - High bonding capacity of the electrode atom to several Li atoms – similar to silicon