Comparison of “natural” Li diffusion behavior into different materials: TiO2/Si(111), TiO2, SrTiO2

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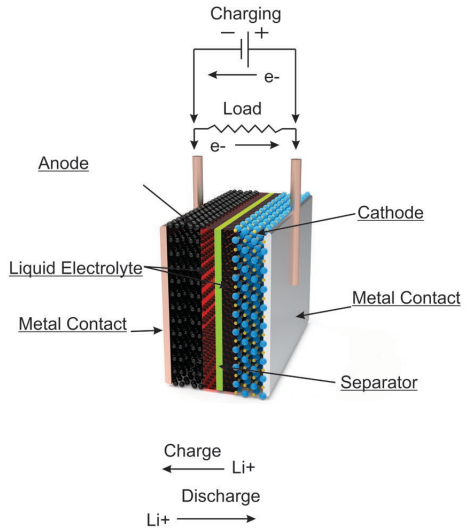
Objective: *Search for the materials that are attractive to “natural“ Li diffusion*

Li transport properties – a key factor for LIB battery performance

Liquid Electrolyte Battery Cell

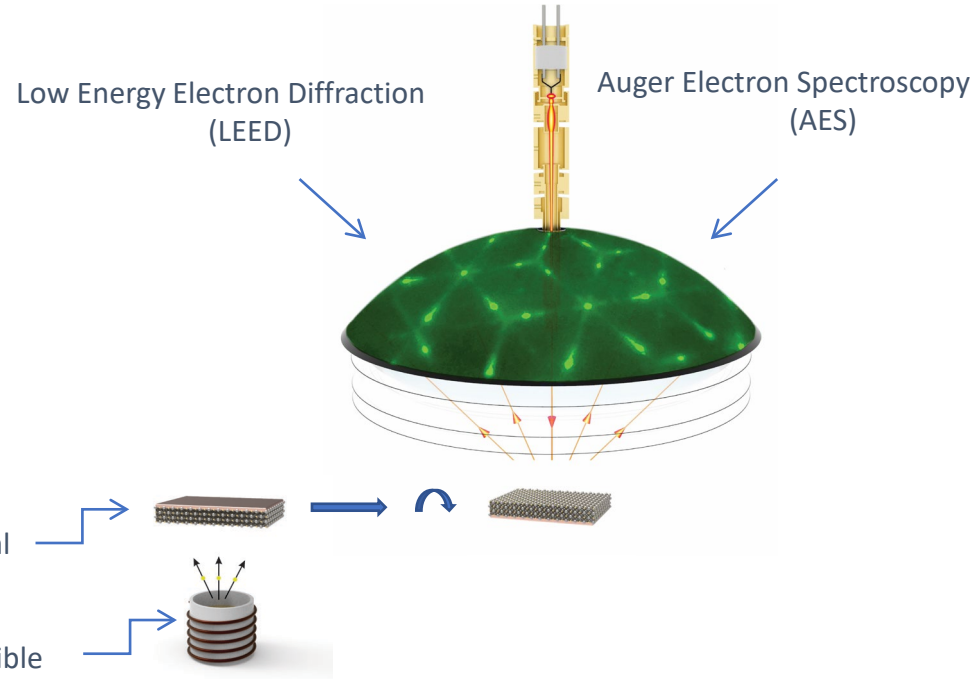


“Natural” Li diffusion:
- Gradient of Li concentration on the surface
- Thermal energy at room temperature
- No external electrical potential

Electrodes with high “natural” Li diffusion will perform better in LIB applications because there is another component for the atomic migration such as lattice

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

Method:- *Evaporation of ultra-thin film of Li*
- Li concentration tracing with AES (KVV 52eV)
- Surface crystallography monitoring with LEED



! Novel Methodology !

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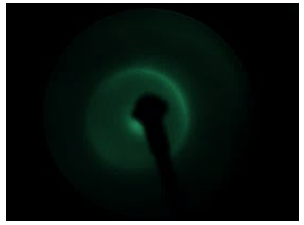
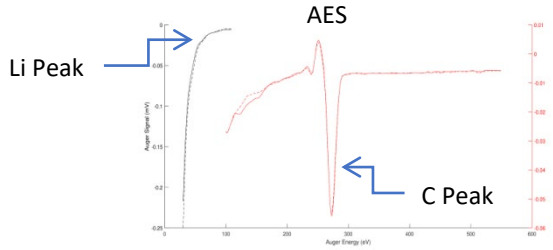
LEED and AES Data & Conclusions

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

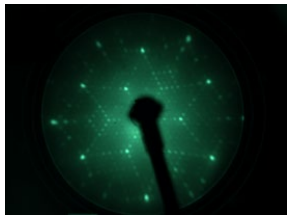
Before Lithium Evaporation

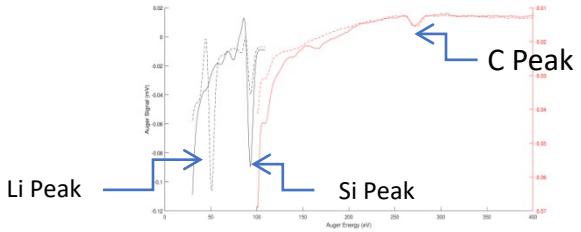
5Å Lithium Evaporation



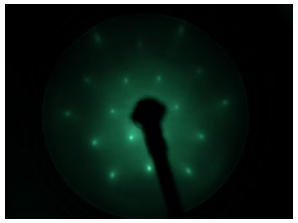


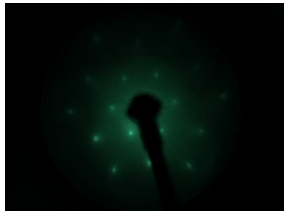
Si(111) – no Li diffusion, drastic change to surface crystalline structure

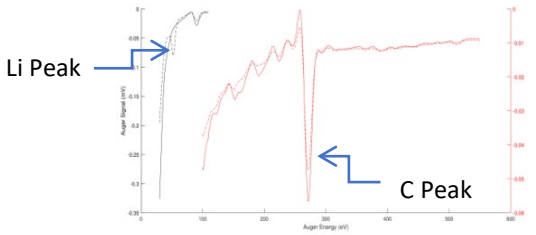




SiC-6H – some Li diffusion, small effect on surface crystalline structure

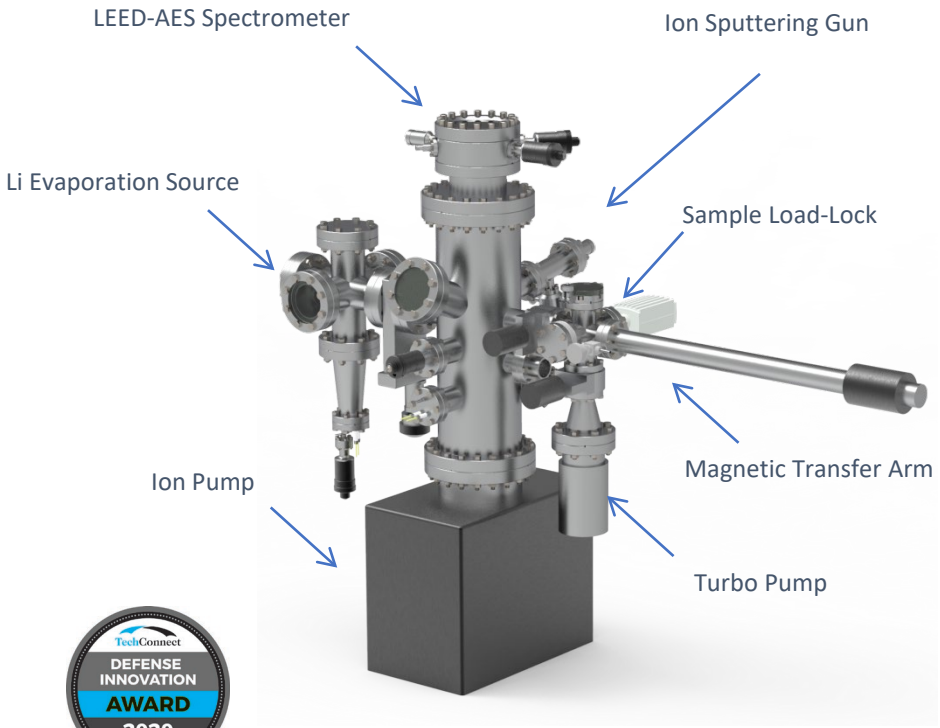






UHV System for Li thermal diffusion tests

- early indicator of battery materials performance



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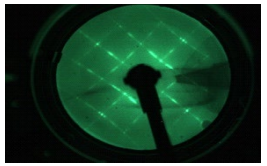
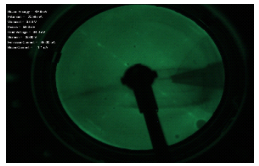
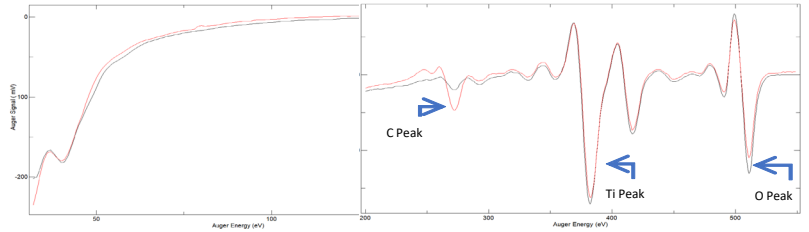
TiO_2 (Titanium Dioxide) – Li diffusion, crystalline structure is affected

Before Lithium Evaporation

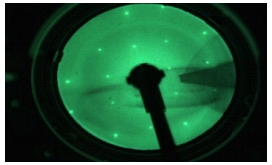


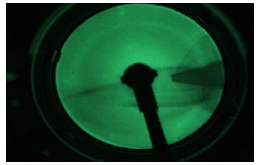
After 10Å of Lithium Evaporation

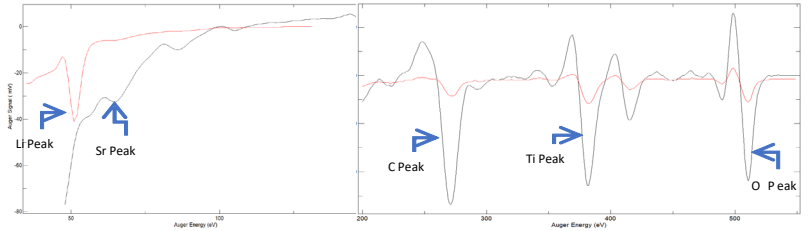




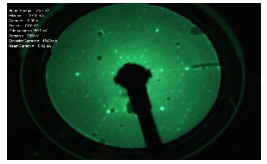
$SrTiO_3$ (Strontium Titanate) – no Li diffusion, crystalline structure is affected

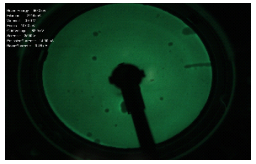


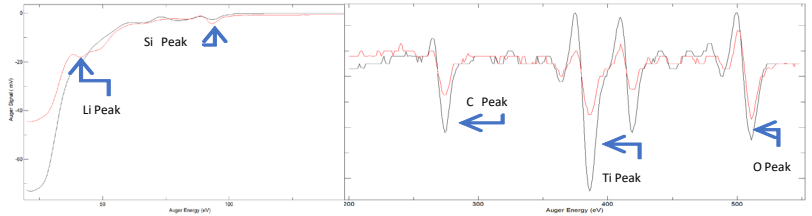




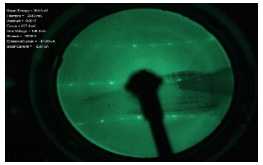
TiO_2 /Si (111) – good Li diffusion, crystalline structure is affected

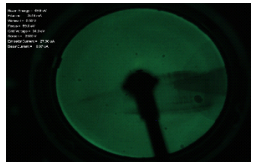


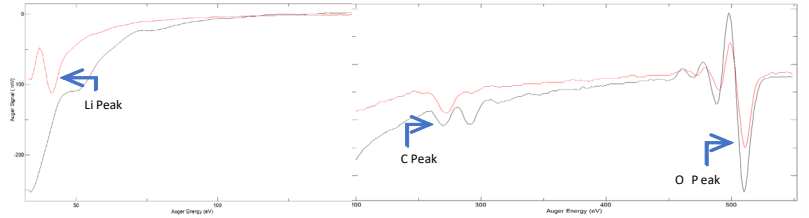




Ga_2O_3 (Gallium Oxide) – no Li diffusion, crystalline structure is affected







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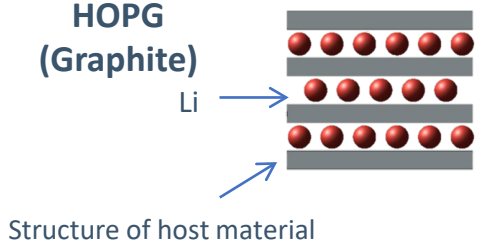
Conclusions

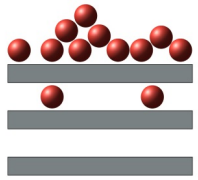
We identified 3 categories of characterized materials:

HOPG (Graphite)



“Rapid lattice diffusion”: Materials with “natural” rapid Li diffusion in lattice structure: HOPG and no effect on long range structural order

Si(111)

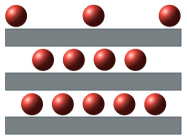


“No lattice diffusion”: Materials with no “natural” Li diffusion and a strong effect on long range structural order – polycrystalization or amorphization

Si(100), Si(211), SrTiO2, Ga2O3

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

SiC-6H



“Moderate lattice diffusion”: Materials that have moderate “natural” Li diffusion and some effect on the long range structural order

SiC, CVD Diamond, LiNb2O3, TiO2, TiO2/Si(111)

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Conclusions

- So far, we didn’t find material with similar diffusion properties as HOPG and Graphite
- These materials with moderate lattice diffusion can’t be used as a replacement for graphite, but they can improve the graphite interface for chemical stability at the solid-electrolyte interface or collector-anode interface.
- Silicon lattice is presenting the barrier for Li lattice diffusion. Silicon is a very attractive material because of its high capacity for bonding with Lithium. However, the lack of lattice diffusion requires to develop of special structural paths allowing migration of Li atoms/ions
- Ga2O3 is a wideband semiconductor with a layered structure bonded together with van der Walls forces. However, this layered structure is not contributing to Li lattice diffusion.

Techniques:

- Auger electron spectroscopy (AES) and Low energy electron diffraction (LEED) are very powerful tools for characterizing passive Li diffusion in the wide range of materials