



Atomic Layer Deposition: Past, Present, and Future

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Company Overview – PneumatiCoat (PCT)

- Technology
 - Improve pack performance and cost using encapsulation coatings that deliver sustainable \$/kWh advantages
- Value Proposition
 - Increased performance
 - Lower cost per kWh
- Atomic Layer Deposition (ALD)
 - Toll Coating
 - Service Contracts
 - Production Systems
 - Grant Opportunities

PCT's Impact: BRINGING VALUE TO CUSTOMERS AND OEMs

HELPING TO MAKE BATTERIES SMALLER, LIGHTER, SAFER AND CHEAPER



Vision Statement: To be the world leader in innovative materials solutions, and to create safer and more efficient products.

Outline

- Active Materials and Encapsulation Benefits
- Encapsulation Processes and ALD Background
- ALD processing: Current/Future Advantages and Historical Disadvantages
- Capabilities and Demonstrated Benefits of ALD
- Commercial ALD Solutions
- Summary and Recommendations





Active Materials

• Incremental improvements in quality, energy density over 30 years

The 1980s and 1990s recorded many successful discoveries and the commercialization of oxide-based cathode materials such as the layered compounds $LiCoO_2$, $LiNiO_2$, spinel $LiMn_2O_4$, and mixed oxides (e.g., $LiMn_{1.5}Ni_{0.5}O_4$, $LiMn_{0.33}Co_{0.33}Ni_{0.33}O_2$, and $LiNi_{0.8}Co_{0.15}Al_{0.05}O_2$) [6–10]. Among the massive research carried out on oxide insertion compounds, in 1997, Padhi et al. introduced the concept of polyanionic compounds as an alternative class of cathodes, $LiFePO_4$ being the first example [11,12]. In the lithium-battery field, the

B. Scrosati et al. Lithium Batteries: Advanced Technologies and Applications. 2013.

- However materials still suffer from *surface-driven degradation*:
 - Electrolyte Interactions
 - Phase Transitions
 - Oxygen Loss
 - Particle Fractionation
 - Conductivity Loss
 - SEI / Resistivity Build-up





Next Gen Performance Requires Coated Particles

KEY PROBLEMS AT 4.5 V CHARGE

Degradation During High
 Temp Storage (60°C, 90°C)
 ➢ Ni⁴⁺, Co⁴⁺ dissolution
 ➢ Accelerated interfacial reactions with electrolytes

Degradation During Cycling

- Anisotropic volume expansion/contraction
- ➢ Ni⁴⁺, Co⁴⁺ dissolution

Degraded Thermal Stability

- Oxygen extraction from lattice
- Exothermic reaction with electrolytes



SOLUTIONS AND CRITICAL TO QUALITY ATTRIBUTES

Adapted from Figure 3 of J. Cho, P.G. Bruce et al., Angew. Chem. Int. Ed. 2012, 51, 9994 – 10024.

Process Windows of Coating Techniques



ALD offers precision control required to prevent resistivity build-up due to coatings

Next Gen Performance Requires Coated Particles

Rough Coating (Co-Precipitation)



Lots of bared area.
Protection was not maximized.

Improved performance deteriorates due to inconsistent coating

Adapted from: Z. Chen, Y. Qin, K. Amine, Y.-K. Sun *J. Mater. Chem.* 2010, **20**, 7606-7612

Core-Shell (Co-Precipitation)



 Coating shell composes of multiple layer of nano particles.

•Thick coating layer impede the transport of electron and Li⁺.

> Thick, consistent coating causes high resistivity

Ultrathin Film Coating (ALD)



- Tunable thickness.
- Complete coating.
- ·Precise control.
- ·Can be obtained by ALD,

Ultrathin consistent coating has lasting performance with no resistivity impacts

Rational Design of Optimal Coatings

Quantum simulation of oxides:

- Single non-porous monolayer is sufficient to mitigate electrolyte degradation
- Chemically bonded film (ALD) is the most durable solution
- Simple ALD coatings can lithiate and fluorinate in situ
- Complex ALD coatings further enhance thermal, mechanical and electrochemical stability





Courtesy of C. Musgrave University of Colorado at Boulder



Overview of ALD Process



Direct technology comparison: Li-ion Batteries

Material efficiency is the difference









ALD delivers <u>improved</u> long-term performance at <u>reduced</u> material costs

US Patent 8,993,051

ALD provides enhancements to ALL chemistries

Particle ALD delivers clear, low-cost value propositions for all market applications

- Increased capacity retention
- Higher temperature stability
- Greater over-voltage protection
- Faster charge/discharge rates
- Reduced Cost of Ownership

ALD Ultrathin Al₂O₃ ALD



120

Clear scale-up roadmap: High throughput spatial ALD processing system for particles

The Challenge: No silver bullet coating, all must be optimized by type



References for Scott et al, Jung et al., Riley et al., available upon request 11

High Temperature Performance and Safety

- High temperature performance
 - Demanding applications
 - Reduced cooling requirements

- Safety Improvements
 - Exothermal reaction temperature increased by 40°C



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Energy Storage Benefits of ALD



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Common ALD Techniques

- Lithium-ion Batteries
 - Particle vs. Electrode
- Particle ALD
- Electrode ALD



Particle - Fluidized Bed



Electrode - Batch



Electrode – R2R





Particle – Semi-continuous

High Throughput Spatial ALD (Particle)



- Excellent process control
- Throughput independent of number of cycle
- Scalable



High Throughput Spatial ALD (Particle)

PROTOTYPE SCALE (3 kg/hr)



Particle Advantages

- Cost Effective
- Drop in (front-end or back-end)
- Excellent quality control
- Near-Zero waste
- Demonstrated throughput
- Robust coatings







Particle ALD Commercial Roadmap



Example Business Case

ALD Improvement	Comparison –	Tesla Battery Co	ost Reduction in	\$/kWh/cycle
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	Target	Base Technology	Proven ALD improvement
		Pack Level: \$120/kWh @ 300 cycles = \$0.40/kWh/cycle	Pack Level: \$120/kWh @ 625 cycles = \$0.19/kWh/cycle
\$/kWh/cycle	Tesla 80 kWh of 4.8 Ah NCA cells	Cathode Level: Sumitomo NCA (195 mAh/g, 3.7V nom., \$25?/kg), 300 cycles = \$0.116/kWh/cycle	Cathode Level: ALD-coated NCA (190 mAh/g, 3.7V nom., \$31/kg], 625 cycles at 4.3V = \$0.071/kWh/cycle Additional energy gain anticipated using higher purity Sumitomo NCA.

- ALD-enabled cathodes show lifetime benefit and higher capacity (range)
- Can reduce Tesla's \$/kWh/cycle by > 50%

Summary

- Raw materials can be significantly improved with surface coatings
- ALD is an ideal tool for improving and optimizing raw materials
- Particle ALD is only viable means towards commercialization
 - Demonstrated 200kg/day
 - Excellent nail penetration data in 40Ah packs
 - Excellent electrochemical performance in 95Ah packs
 - Overall pack cost reduced, at scale
- ALD also has many applications outside of batteries

Particle ALD Products and R&D Opportunities





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Thank you

- Special thanks to the Vehicle Technologies Office (VTO) SBIR Phase I/II program DE-SC0010230 for supporting ALD cathode scale-up efforts
- New DOE (VTO) SBIR Phase I program for ALD-enabled anodes
- Other DOE, Navy, Air Force SBIR programs through additional primary or subcontract awards

Questions



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Commercializing "nano"

Systems and Technology

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Battery Example 1 : NCA

Low-Gassing PICOSHIELD® NCA – coarse and fine grades



Benefits include:

Reduced gassing Longer lifetime Higher stability at higher voltages Drop-in ready









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Battery Example 2 : NMC

Long-Life PICOSHIELD® NMC – many compositions



<u>Benefits include:</u> Longer lifetime Increased Safety Higher voltage stability







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Battery Example 3 : LMNO

Long-Life PICOSHIELD® MNO – many compositions



