



ES240 Final Project

Intercalation-induced stress in amorphous Si thin film anode of Li-ion Battery

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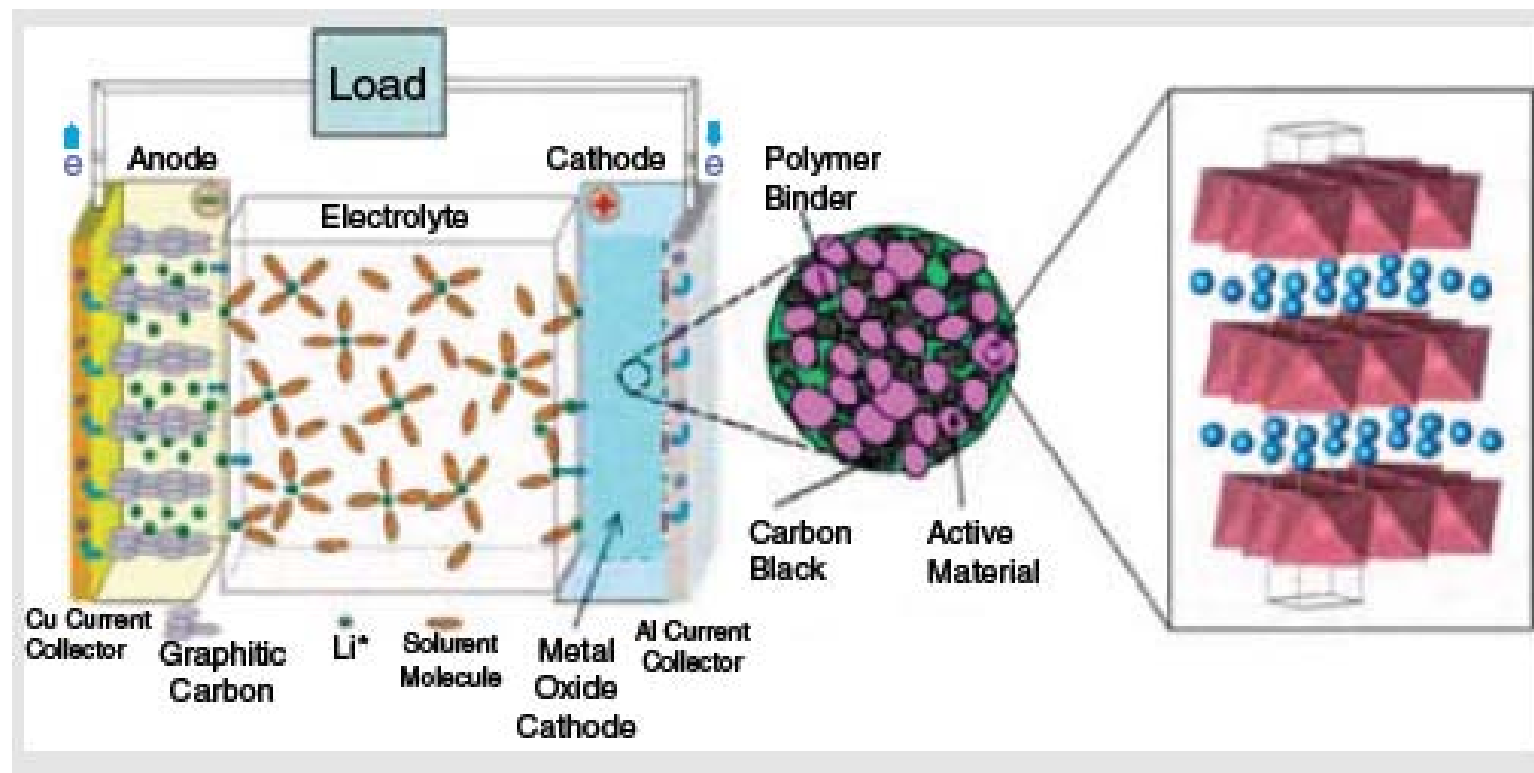
12/09/08

Harvard School of Engineering and Applied Science

Layout

- What is battery?
- What happened in Si thin film anode?
- Simulation results

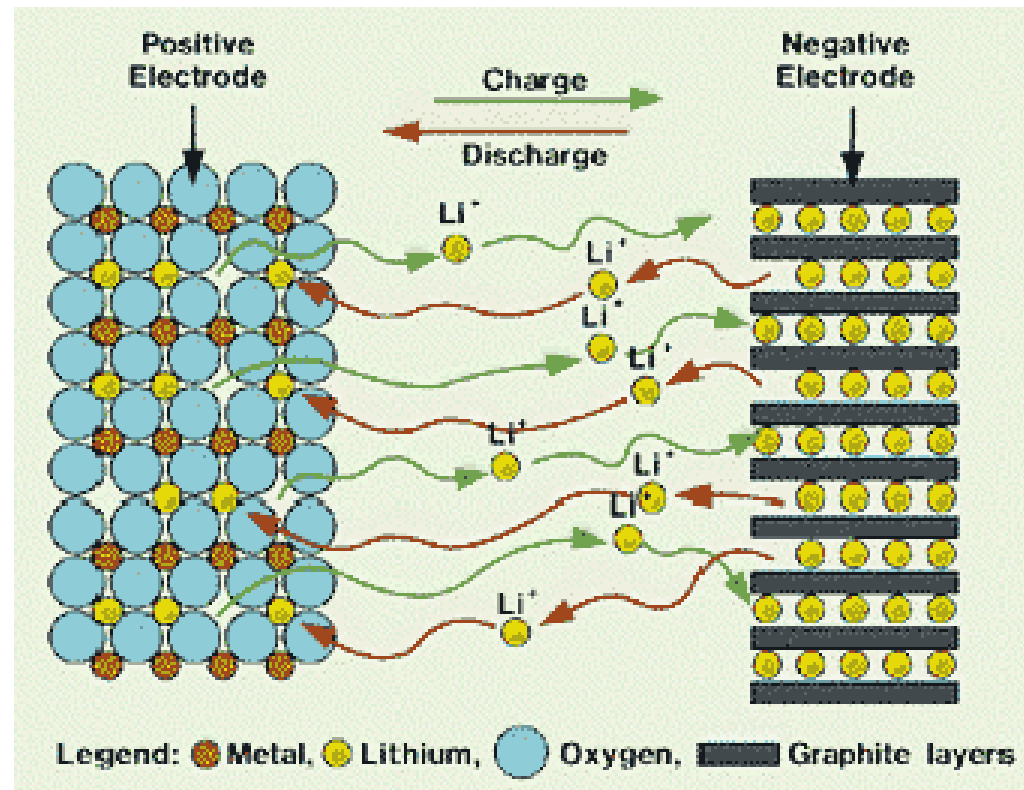
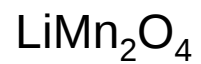
What is Battery?



M. Stanley Whittingham. MRS Bulletin. 33,2008

Lithium-ion Battery

Cathode



Anode

C_6 (graphite)

Si

CNTs

Si-NWs

Lithium-ion Battery

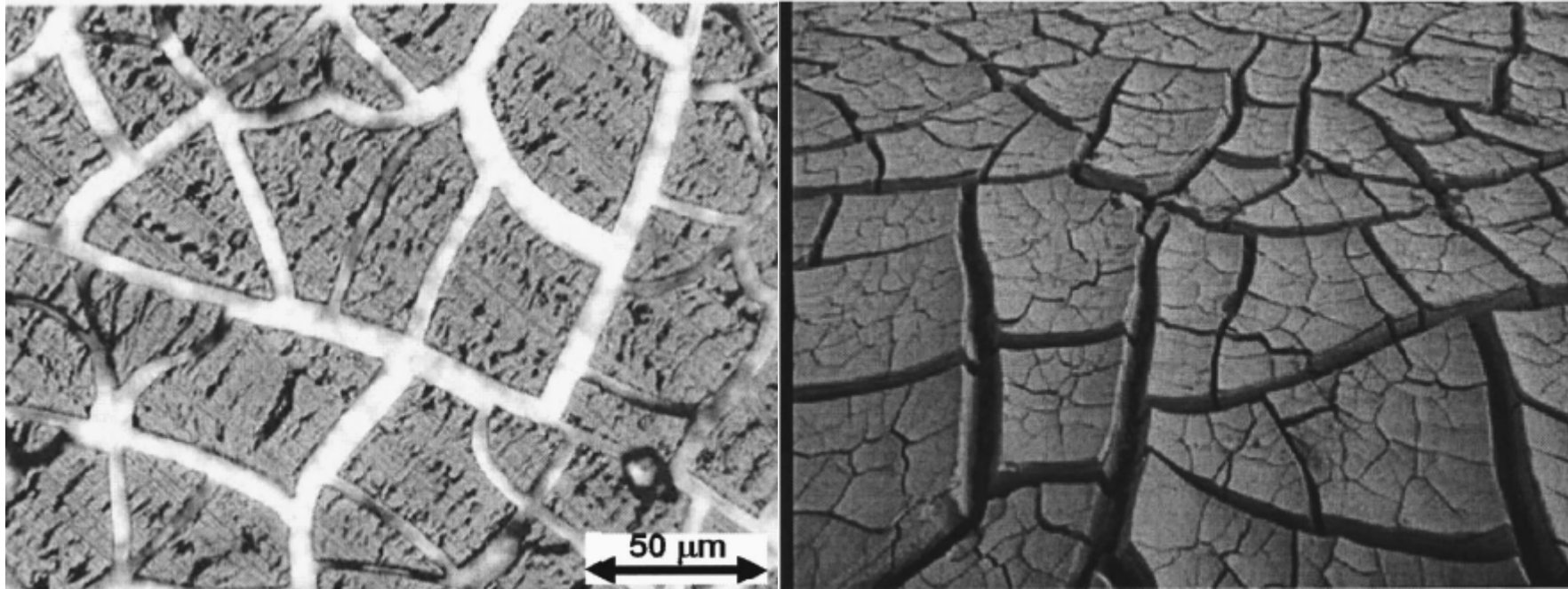


Chevy Volt By General Motors



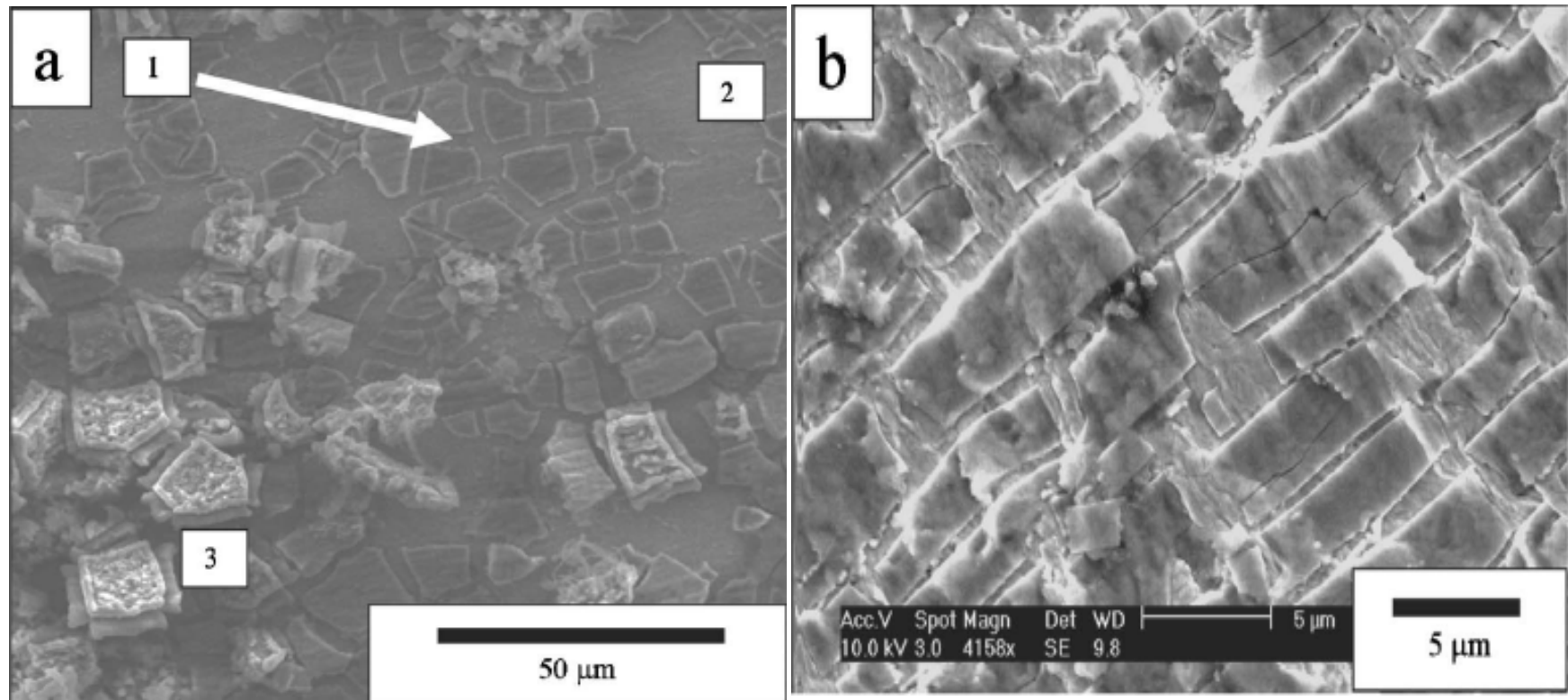
Telsa Roadster By Telsa Motors

Si-based thin film anode



L.Y.beaulieu etc.,Electrochem. Solid-state Lett.,4(9),2001

Si-based thin film anode



J.P.Maranchi etc., J.Electrochem.Soc., 153(6), 2006

Numerical Simulation- *case 1*



ODB: 3D-symmetry.odb Abaqus/Standard Version 6.8-1 Sat Dec 06 08:23:31 Eastern Standard Time 2008



Step: Step-1
Increment 16: Step Time = 6.7663E-02

	Young's Modulus	Poisson's Ratio
Amorphous Si	80GPa	0.22
Polycrystalline Cu	130GPa	0.3

$$\frac{T_f}{T_s} = 1, \quad \frac{\text{Thickness}}{\text{Radius}} = \frac{1}{100}$$

Numerical Simulation- *case 1*



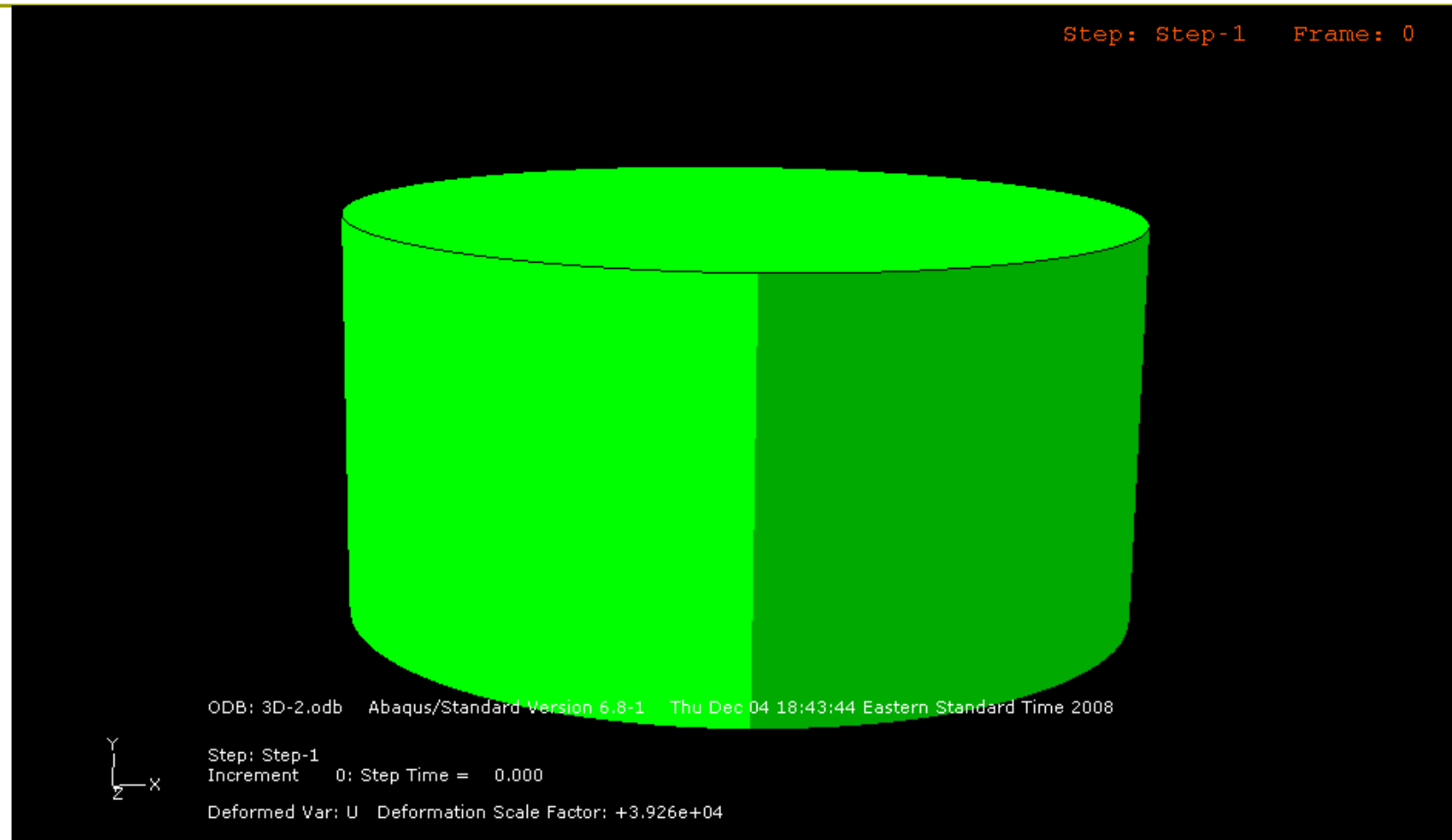
Analysis

Material's Law:
$$\varepsilon_{ij} = \frac{1}{E}[(1 + \nu)\sigma_{ij} - \nu\sigma_{kk}\delta_{ij}] + \alpha\Delta T$$

Stoney formula:
$$k = \frac{12\varepsilon_m M_f}{h_s M_s} \left[1 + 14 \frac{M_f}{M_s} + \left(\frac{M_f}{M_s} \right)^2 \right]^{-1}$$

Error = 1.07 %

Numerical Simulation- *case 2*



Mises Stress in the thin film, $S=300\text{GPa}$

Numerical Simulation- *case 3*

Material's Law:

Thin film: Deformation plastic

$$E\varepsilon = \sigma + \alpha \left(\frac{\sigma}{\sigma_0} \right)^2 \sigma$$

Substrate: Elastic

Mises Stress in thin film: $S=15\text{GPa}$

Conclusions

- The intercalation-induced stress is high enough to crack the amorphous Si thin film
- Fracture/debonding dominate the failure of thin film anode in Li-ion battery



Thank you!

To see a world in a grain of sand
And a heaven in a wild flower
Hold infinity in the palm of your hand
And eternity in an hour