OOF Extensions and Applications to Multifunctional Materials and Devices: An Overview

R. Edwin García
Energy Materials

Outline

Current Research

- Rechargeable batteries
- Piezoelectrics and electrostrictors
- Light emitting devices
- Ferroelectrics

Actuator Materials
Rechargeable Lithium-Ion Batteries

Yet-Ming Chiang, W. Craig Carter

\[
\frac{\partial c}{\partial t} = \nabla \cdot (D_L \nabla c) + \nabla \cdot (L \nabla \phi)
\]

**diffusion term**

**ohmic term**

\[
\theta = \nabla \cdot (\rho \nabla \phi) + \nabla \cdot (L \nabla c)
\]

**elastic fields**

\[
\sigma_{ij} = C_{ijkl} (\varepsilon_{kl} - \beta_{kl} (c - c_0))
\]

\[
\nabla \cdot \sigma = 0
\]

**electromigration terms**

\[
0 = \nabla \cdot (\rho \nabla \phi)
\]

**ohmic load**

\[
\vec{J} \cdot \hat{n} = J_o \left( e^{\frac{\alpha_a F \eta}{RT}} - e^{\frac{\alpha_c F \eta}{RT}} \right)
\]

**graphite**

**LiMn_2O_4**
Model Validation: Comparison with Experiment

Experimental Data: Christopher Marc Doyle “Design and Simulation of Lithium Rechargeable Batteries.” PhD thesis, Department of Chemical Engineering, University of California at Berkeley, 1995
Initial Stages of Battery Discharge

Lithium concentration (normalized)

0.3
0.17

1s
10s
15s
20s
Late Stages of Voltage Distribution of Battery Discharge

Full Battery Microstructure

Voltage Distribution (Volts)

1C: 2.0 mA/cm²
Late Stages of Battery Discharge

Lithium concentration (normalized)

Voltage distribution

3200 s
3210 s
3220 s
Galvanostatic Discharge Stresses

cathode microstructure

hydrostatic stresses

lithium concentration
Summary Ragone Plot of Mixed Rocking Chair Batteries

Specific Energy (W h/kg)

Specific Power (W/kg)

graphite
LiCoO$_2$
LiMn$_2$O$_4$
Advanced Rechargeable Batteries

Graphite \( \text{LiMn}_2\text{O}_4 \)
depleted after 250s

I=80 A/m²
Summary Ragone Plot of Rocking Chair Batteries

Specific Energy (W h/kg)

Specific Power (W/kg)

- graphite
- LiCoO$_2$
- LiMn$_2$O$_4$
Mass Diffusion Equation
Charge Continuity Equation
Heat Diffusion Equation
Electrochemical Couplings
Time-Stepper Methods
GMRES Solver
Multimeshing Techniques
Line (Interfacial) Elements
Stress Engineering of Light Emitting Devices

(Parijat Deb, Tim Sands)

Crystallography of GaN Pyramids
Elastic Energy Density Distribution

\[ \text{Elastic energy density (J/m}^3) \]

Distance (m)

\[ 0 \text{ J/m}^3 \to 10^8 \text{ J/m}^3 \]

\[ [0001] \]

\[ \text{In}_{0.2}\text{Ga}_{0.8}\text{N} \]

GaN

25 nm
Strain Energy Density

Thin film

Nanowire (50 nm dia.)

Misfit dislocation configuration

Nanorod with pointed tip morphology

Underlayer (U) $\rightarrow$ GaN
Overlayer (O) $\rightarrow$ In$_{0.2}$Ga$_{0.8}$N

Dislocation Energy for a 50 nm nanowire ($\sim$0.2 J/m$^2$)

Energy Density (J/m$^2$)

Overlayer thickness (nm)
Embedded Quantum Well Heterostructure

Zero strain energy density

Energy density (J/m³)

Distance (nm)

GaN

In₀.₂Ga₀.₈N

2 * 10⁷ J/m³

5 * 10⁷ J/m³

10⁸ J/m³

10⁷ J/m³

10⁶ J/m³

10⁵ J/m³

10⁴ J/m³

10³ J/m³

10² J/m³

10¹ J/m³

0 J/m³

0 J/m³
Energy Materials

Outline

- rechargeable batteries
- light emitting devices
- piezoelectrics and electrostrictors
- ferroelectrics

Actuator Materials
Polycrystalline PZT Film

2 $\mu$m
The Piezoelectric Solid

Converse piezoelectric effect

Direct piezoelectric effect

Higher order piezoelectric response

Electromechanical Helmholtz free energy

\[ f = u - \bar{D} \cdot \bar{E} \]

\[ f = \frac{1}{2} \sigma \cdot \varepsilon - \frac{1}{2} \bar{D} \cdot \bar{E} \]

\[ \nabla \cdot \bar{D} = 0 \]

\[ \nabla \cdot \sigma = 0 \]
Simulation of Polycrystalline PZT Films

\[ \nabla \cdot \vec{D} = 0 \]

\[ D_i = \epsilon_{ij} E_j + d_{ikl} \sigma_{kl} \]

\[ \sigma_{ij} = C_{ijkl} (\varepsilon_{kl}^T - d_{ikl} E_i - \alpha_{kl} \Delta T) \]

\[ \frac{\partial P}{\partial t} = -M \frac{\delta F}{\delta P} \]
Piezoelectric Force Microscopy of Ferroelectric Films
Virtual Piezoelectric Force Microscopy of Ferroelectric Films

2 μm diameter probed area
Polarization (C/m$^2$)

Electric Field (V/m)

Polarization (C/m$^2$)

Electric Field (V/m)
0.25 C/m²

out-of-plane polarization

0.27 C/m²

polarization vector magnitude

0.24 C/m²

0.25 C/m²

-0.25 C/m²

out-of-plane polarization

30 µm

001 010 110

x y z
Coulomb’s Equation
Piezoelectric Couplings
Non-Linear Solvers
Elementary Adaptive Meshing Tools
Ferroelectricity
Runge-Kutta Solvers
Predictor-Corrector Method
Energy Materials

Outline

- rechargeable batteries
- light emitting devices
- solid oxide fuel cells
- piezoelectrics and electrostrictors
- ferroelectrics
- solid oxide fuel cells
- thermoelectric generators

Research
# Credits

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<tr>
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<th>Contributors</th>
<th>Institution</th>
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<tbody>
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<td>InGaN Light Emitting Devices</td>
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