

ELECTRIC VEHICLE BATTERIES R&D

2001
ANNUAL
PROGRESS
REPORT



U.S. Department of Energy
Energy Efficiency and Renewable Energy
Office of Transportation Technologies

A C K N O W L E D G E M E N T

We would like to express our sincere appreciation to Energetics, Inc., and to Argonne National Laboratory for their artistic and technical contributions in preparing and publishing this report.

In addition, we would like to thank all our program participants for their contributions to the programs and all the authors who prepared the project abstracts that comprise this report.

**U.S. Department of Energy
Office of Advanced Automotive Technologies
1000 Independence Avenue S.W.
Washington, D.C. 20585-0121**

FY 2001

**Progress Report for the Electric Vehicle
Battery Research and Development Program**

**Energy Efficiency and Renewable Energy
Office of Transportation Technologies
Office of Advanced Automotive Technologies
Energy Management Team**

Raymond A. Sutula

Energy Management Team Leader

December 2001

CONTENTS

	<u>Page</u>
1. INTRODUCTION	1
2. ELECTRIC VEHICLE BATTERY RESEARCH AND DEVELOPMENT PROGRAM AND FY 2001 HIGHLIGHTS	3
A. Electric Vehicle Battery Research and Development Program.....	3
3. LITHIUM ION BATTERY DEVELOPMENT	7
A. SAFT Lithium Ion Energy Storage Technology	7
4. BENCHMARK TESTING OF ADVANCED ELECTRIC VEHICLE BATTERIES	11
A. Benchmark Testing Program.....	11
5. INTERAGENCY WORKSHOPS ON ADVANCED BATTERY TECHNOLOGIES	13
A. Workshop on Interfaces, Phenomena, and Nanostructures in Lithium Batteries	13
B. Workshop on Development of Advanced Battery Engineering Models	19
6. ADVANCED BATTERY READINESS WORKING GROUP	25
A. Advanced Battery Readiness Ad Hoc Working Group (ABRWG) Meeting	25
APPENDIX: ABBREVIATIONS, ACRONYMS, AND INITIALISMS	29

1. INTRODUCTION

Electric Vehicle Battery Research and Development Program

The Electric Vehicle Battery Research and Development Program has been a part of the Office of Advanced Automotive Technology since its inception in the late 1970's. Advanced batteries have been an integral part of the high-risk/high payoff activities sponsored by the Department on electric vehicles R&D. The program supports development of battery technologies that would enable commercially competitive electric vehicles. The current goal is to achieve this by the 2005 to 2008 time frame.

The Electric Vehicle Battery Research and Development Program has had several major successes. It successfully developed and introduced the nickel metal hydride advanced battery for electric vehicle use. Over 1000 nickel metal hydride battery electric vehicles have been put into service in the last few years. The program has also conducted the Advanced Battery Readiness Working Group for a decade. The Advanced Battery Readiness Working Group meets regularly to address regulatory issues concerning the shipping, in-vehicle safety, and recycling or reclamation of advanced batteries. This group has created or motivated the creation of new regulations that support the use of advanced battery technologies for hybrid and electric vehicles.

The Electric Vehicle Battery Research and Development Program also conducts extensive benchmarking activities of advanced batteries from abroad. Current work in benchmarking nickel metal hydride battery modules is being expanded to benchmark lithium ion systems (at the cell level).

Advanced batteries remain a key critical technology for the commercialization of electric vehicles. The development of advanced batteries is carried out by the United States Advanced Battery Consortium (USABC). USABC has nearly a decade of experience in managing advanced battery development programs with the Department of Energy for both electric and hybrid electric vehicles. It conducts the world's largest research and development efforts for advanced automotive batteries. It is generally recognized as the leading advanced battery development effort on a world-wide basis.

This report highlights the activities and progress achieved during FY 2001 under the Electric Vehicle Advanced Battery Program. This report consists of program summaries from the major development efforts in this program. The information presented here only reflects what appears in the public domain and does not include any "Protected Battery Information."

Tien Q. Duong
Program Manager
Office of Advanced Automotive Technologies
Office of Transportation Technologies
Department of Energy

2. ELECTRIC VEHICLE BATTERY RESEARCH AND DEVELOPMENT PROGRAM AND FY 2001 HIGHLIGHTS

A. Electric Vehicle Battery Research and Development Program

Ken Heitner

U.S. Department of Energy

EE-32, Room 50-030

Washington, DC 20585-0121

(202) 586-2341, fax: (202) 586-1600, e-mail: kenneth.heitner@ee.doe.gov

Thomas J. Tartamella

Chairman, Technical Advisory Committee

United States Advanced Battery Consortium

(248) 838-5337, fax: (248) 838-5338, e-mail: tt4@daimlerchrysler.com

The Electric Vehicle Battery Research and Development Program was established to develop advanced batteries capable of meeting the industry's long-term goals. The long-term goals were set to enable fully competitive electric vehicles in response to the Zero Emission Vehicle program began in California in 1990. Zero emission vehicles continue to be sought in California and the Northeast to mitigate severe criteria pollutant emissions from mobile sources.

The goal of the Electric Vehicle Battery Research and Development Program [1-4] is to support the development of a domestic advanced battery industry that will allow fully competitive electric vehicles by the 2005 to 2008 time frame. The technical objectives of the program are defined in Table 1.

The Electric Vehicle Battery Research and Development Program is organized as follows:

- The Department of Energy serves as the overall program manager.
- The United States Advanced Battery Consortium conducts cost shared development of advanced batteries with competitively selected developers. The Department of Energy is substantially involved in the management of the USABC and participates in its Management Committee, Technical Advisory Committee, and work groups.
- The USABC also closely follows the work performed by the Batteries for Advanced Transportation Technologies program and other elements of the work of the Energy Management Team. The USABC is also responsible for High Power Energy Storage Program in support of the Partnership for a New Generation of Vehicles.
- The USABC conducts the development of lithium ion batteries.
- The Department of Energy also manages the Benchmark Testing of Advanced Electric Vehicle Batteries.

Table 1. U.S. Advanced Battery Consortium Goals for Electric Vehicle Batteries

Primary criteria	Long-term goals^a (2005 to 2008)
Power density, W/L	460
Specific power, W/kg (80% DOD/30 sec)	300
Energy density, Wh/L (C/3 discharge rate)	230
Specific energy, Wh/kg (C/3 discharge rate)	150
Life (years)	10
Cycle life, (cycles) (80% DOD)	1000 1,600 (@ 50% DOD) 2,670 (@ 30% DOD)
Power and capacity degradation ^b (% of rated spec)	20%
Ultimate price ^c (\$/kWh) (10,000 units @ 40 kWh)	<\$150 (desired to 75)
Operating environment	-30EC to 65EC
Recharge time ^b	< 6 hours
Continuous discharge in 1 hour (no failure)	75% (of rated energy capacity)
Secondary criteria	Long-term goals (2005 to 2008)
Efficiency ^b (C/3 discharge and C/6 charge) ^d	80%
Self-discharge ^b	<20% in 12 days
Maintenance	No maintenance. Service by qualified personnel only.
Thermal loss ^b	Covered by self-discharge
Abuse resistance ^b	Tolerant Minimized by on-board controls
Specified by contractor Packaging constraints Environmental impact Safety Recyclability Reliability Overcharge/over-discharge tolerance	

^a For interim commercialization (reflects USABC revisions of September 1996).
^b Specifics on criteria can be found in *USABC Electric Vehicle Battery Test Procedures Manual, Rev. 2*, DOE/ID-10479, January 1996.
^c Cost to the original equipment manufacturers.
^d Roundtrip charge/discharge efficiency.

Significant Accomplishments for FY 2001

During FY 2000, the Department of Energy awarded USABC a Phase III cooperative agreement covering the period March 2000 to June 2003. That agreement was for \$62 million dollars, with a cost share of 35 percent from the Department of Energy and 65 percent from industry.

The USABC is committed to continue work on lithium ion batteries. The USABC is also evaluating lithium “gel” polymer batteries and may consider other lithium based battery technologies in the future. In June 2001, the USABC issued a Request For Proposal Information (RFPI) entitled “PNGV Development of Low-cost Separators For Lithium-ion Batteries”.

The USABC continues to cooperate with the Lithium Battery Energy Storage Research Association of Japan (LIBES) under agreements signed in 1998 between the Department of Energy and the Japanese Ministry of International Trade and Industry. This cooperation is focused at methods for electric testing and tolerance to abuse testing of lithium batteries. Both sides also are exploring ways in which the battery users and developers can work more closely to understand the needs of the market and offer appropriate prototype technology for evaluation.

The Benchmark Testing of Advanced Electric Vehicle Batteries Program is continuing to test electric vehicle nickel metal hydride modules and is beginning to evaluate electric vehicle lithium ion and lithium polymer cells being received from overseas developers.

Program Participants

The FY 2001 participants in this program are:

- United States Advanced Battery Consortium
- AVESTOR (subsidiary of Hydro-Quebec)
- SAFT (France)
- Argonne National Laboratory

References

- [1] Sutula, R.A., Heitner, K.L., Rogers, S.A., Duong, T.Q., Kirk, R.S., Kumar, B., and Schonefeld, C., "Electric and Hybrid Vehicle Energy Storage R&D Programs of the U.S. Department of Energy," the 16th International Electric Vehicle Symposium, Beijing, China, October 1999.
- [2] Sutula, R.A., Heitner, K.L., Rogers, S.A., Duong, T.Q., Kirk, R.S., Kumar, B., and Schonefeld, C., "Advanced Automotive Technologies Energy Storage R&D Programs at the U.S. Department of Energy: Recent Achievements and Current Status," paper No. 2000-01-1604, the 2000 Future Car Congress, Arlington, VA, April 2000.
- [3] Sutula, R.A., Heitner, K.L., Rogers, S.A., Duong, T.Q., Kirk, R.S., Battaglia, V., Henriksen, G., McLarnon, F., Kumar, B., and Schonefeld, C., "Recent Accomplishments of the Electric and Hybrid Vehicle Energy Storage R&D Programs at the U.S. Department of Energy: A Status Report," the 17th International Electric Vehicle Symposium, Montreal, Canada, October 2000.
- [4] Sutula, R.A., Heitner, K.L., Barnes, J.A., Duong, T.Q., Kirk, R.S., Battaglia, V., Kumar, B., and Schonefeld, C., "Current Status Report on U.S. Department of Energy Electric and Hybrid Electric Vehicle Energy Storage R&D Programs," the 18th International Electric Vehicle Symposium, Berlin, Germany, October 2001.

3. LITHIUM ION BATTERY DEVELOPMENT

A. SAFT Lithium Ion Energy Storage Technology

Tien Q. Duong

U.S. Department of Energy

EE-32, Room 5G-030

Washington, DC 20585-0121

(202) 586-2210, fax: (202) 586-1600, e-mail: tien.duong@ee.doe.gov

Ahsan Habib

U.S. Advanced Battery Consortium

(248) 680-5946, fax: (248) 680-5131, e-mail: ahsan.habib@gm.com

Objectives

- Develop a lithium ion battery system for electric vehicle that can meet the required high performance levels for energy and power, has a long life, a low cost, and is tolerant of abuse.

Approach

- Adopt a cylindrical form factor.
- Internally connect cells in various fixed, series and parallel configurations to obtain a voltage design flexibility.
- Engineer technology based on existing and emerging battery materials available from international suppliers.

Accomplishments

- Continued to obtain improved performance levels for lithium ion cell technology.

Future Directions

- Continue development of the cell technology and module and pack level technology.

Since they were first introduced in the early 1990's, lithium ion batteries have enjoyed an unprecedented growth and success in the consumer marketplace. The current SAFT Lithium Ion electric vehicle cell technology has evolved from programs initiated in 1993 in Europe. Today several vehicles are being road tested in Europe using lithium ion batteries. As part of this evolution, SAFT has developed an integrated modular concept to provide design flexibility and packaging efficiency. With abuse tolerance being a primary objective of the program, the batteries currently being tested have

demonstrated an energy density of 125 Wh/kg at the battery level. Figures 1 and 2 show the family of High Energy (HE) and High Power (HP) lithium ion cells and EV module package.

Performance

Table 1 shows the lithium ion cell performance data. A summary of the performance for the HE Lithium Ion chemistry at the module level appears in Table 2.



Figure 1. Lithium ion family of cells and EV module

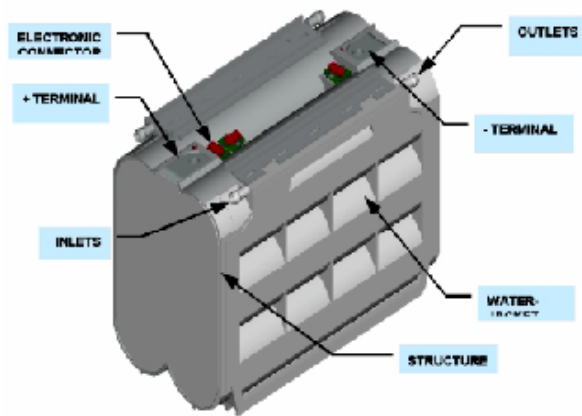


Figure 2. High energy module

Abuse Tolerance

For any EV battery system to be utilized in a commercial vehicle, it must not only provide acceptable performance at affordable pricing, but must also exhibit acceptable tolerance to abuse conditions. The SAFT HE lithium ion batteries have been tested for abuse tolerance during their development.

Future Development

As an ongoing program, the objectives are to simultaneously improve performance while concurrently driving down the cost of manufacturing.

Table 1. Lithium ion high energy cell performance [1, 2]

Electrical Characteristics	
Nominal voltage (V)	4.0
Capacity @ C/3 rate (Ah)	42
Specific energy (Wh/kg @C/3)	145
Energy density (Wh/dm ³ @C/3)	302
Specific power (W/kg, 80%DOD @C/3)	270
Power density (W/dm ³)	570
Mechanical characteristics	
Diameter (mm)	54
Height (mm)	220
Weight (g)	1.05
Volume (dm ³)	0.5
Operating conditions	
Operating temperature range (EC) as given by the thermal management system	-10/+45
Transport or storage temperature range (EC)	-40/+65
Voltage limits	
In charge (V)	4
In discharge (V)	2.7

Table 2. Lithium ion high energy module performance [3]

Electrical Characteristics	
Nominal voltage (V)	10.8
Capacity @ C/3 rate (Ah)	84
Specific energy (Wh/kg @C/3)	125
Energy density (Wh/dm ³ @C/3)	190
Specific power (W/kg, 80%DOD @C/3)	240
Power density (W/dm ³)	360
Mechanical characteristics	
Length (mm)	232
Width (mm)	116
Height (mm)	175
Weight (kg)	7.15
Volume (dm ³)	4.7
Operating conditions	
Operating temperature range (EC) as given by the thermal management system	-10/+45
Transport or storage temperature range (EC)	-40/+65
Voltage limits	
In charge (V)	12
In discharge (V)	8.1
Peak at 80% DOD (V)	6.9

References

- [1] Sack, T.T., Saft, M.C., Chagnon, G., Oweis, S., Romero, A., Zuhowski, M., Faugeras, T., Sarre, G., Morhet, P., and d'Ussel, L., "Lithium Ion Energy and Power Storage Technology," paper No. 2000-01-1589, the 2000 Future Car Congress, Arlington, VA, April 2000.
- [2] Blanchard, Ph., Cesbron, D., Rigobert, G., and Sarre, G., "Performance of SAFT Li-ion Batteries for Electric Vehicles," the 17th International Electric Vehicle Symposium, Montreal, Canada, October 2000.
- [3] "High Energy Lithium-ion module for automotive industry," SAFT web site, SAFT Batteries, Bagnole, France, http://www.saftbatteries.com/automotive/uk/datasheet/d2_12.htm.

4. BENCHMARK TESTING OF ADVANCED ELECTRIC VEHICLE BATTERIES

A. Benchmark Testing Program

Tien Q. Duong

U.S. Department of Energy

EE-32, Room 5G-030

Washington, DC 20585-0121

(202) 586-2210, fax: (202) 586-1600, e-mail: tien.duong@ee.doe.gov

Ira Bloom

Argonne National Laboratory

Argonne, IL 60439-4803

(630) 252-4516, fax: (630) 252-4176, e-mail: bloom@cmt.anl.gov

Objectives

- Benchmark developers' technologies as a way of using limited resources for the greatest benefit, allowing DOE to gauge the maturity of certain battery technologies and/or to identify their barriers and guiding DOE to allocate appropriately its research funds to address identified barriers or to support other advanced battery technologies.

Approach

- Conduct effort independently and hold results in confidence between DOE and the developer/supplier.
- Select representative nickel metal hydride and lithium ion battery technologies, intended for electric vehicle (EV) and hybrid-electric vehicle (HEV) applications.
- Perform tests based either on the USABC Battery Test Procedures Manual for EV batteries or on the PNGV Battery Test Procedures Manual (HEV).

Accomplishments

- Batteries representing technologies from foreign developers/suppliers were acquired and tested during fiscal year 2001.

Future Directions

- Continue testing with additional foreign battery technologies focusing on lithium-based batteries.

One of the objectives of DOE's battery testing program is the direct comparison of foreign battery technologies with those developed domestically. To accomplish this objective, batteries representing technologies from foreign developers/vendors were acquired and tested during fiscal year 2001. These batteries are from Panasonic/Matsushita (Japan), and Shin-Kobe (Japan). These batteries are intended for

electric vehicle (EV) and hybrid-electric vehicle (HEV) applications. The tests performed on the batteries are based on the either the USABC Battery Test Procedures Manual for EV batteries [1] or on the PNGV Battery Test Procedures Manual (HEV) [2]. The tests were conducted in the Electrochemical Analysis and Diagnostics Laboratory (EADL) at Argonne National Laboratory.

EV Applications

Shin-Kobe Lithium-Ion EV Cells

These cells are rated at 3.75 V and 90 Ah and are based on lithium-ion technology with manganese dioxide cathodes [3]. The test plan for these cells includes core characterization, 48-h stand test, 80%DOD DST life cycling at 10, 25, 40, and 50°C. These cells are reaching the end-of-test. RPTs were performed to gauge changes in cell performance with time. The RPTs consisted of 100% C/3 discharge, 100% DOD DST discharge and peak power measurements. The RPTs were performed every 50 cycles (~1 per month) during life cycling.

HEV Applications

Panasonic/Matsushita Prismatic Test Pack

The test pack is based on Ni/MH technology and is rated at 144 V and 6.5 Ah [4]. The test plan includes state-of-charge curve measurement, C/1 capacity measurements, low-level hybrid pulse-power characterization (HPPC-L) [2], 1 week stand test at 60% state of charge, and cycle life using the 25-Wh profile¹. The pack is currently performing the cycle life test with RPTs every 20,000 cycles. These RPTs consist of C/1 capacity measurement and an HPPC-L.

Shin-Kobe HEV Cells

These cells are rated at 3.6 V and 3.6 Ah and are based on lithium-ion technology with manganese

dioxide cathode technology. The test plan includes C/1 capacity measurements, low-level hybrid pulse-power characterization (HPPC-L), and cycle life using the 25-Wh profile. The cells are currently performing the cycle life test with RPTs every 20,000 cycles. These RPTs consist of C/1 capacity measurement and an HPPC-L.

The specific data from these tests is the subject of non-disclosure agreements with Argonne National Laboratory. Public data sheets about these batteries [3-5] are generally available from the developer.

References

- [1] USABC Battery Test Procedures Manual, Rev. 2, January 1996, DOE/ID-10479.
- [2] PNGV Battery Test Procedures Manual, Rev. 3, February 2001, DOE/ID-10597.
- [3] Lithium-ion cell data specification sheet, Shin-Kobe Electric Machinery Co., Ltd., Tokyo, Japan.
- [4] Panasonic/Matsushita Test Pack data specification sheet, Matsushita Electric Industrial Co., Ltd., Tokyo, Japan.
- [5] Press Release: Mn type Li-Ion Battery for HEV, Shin-Kobe Electric Machinery Co., Ltd., Tokyo, Japan http://www.shinkobe-denki.co.jp/e/release/release00322_e.htm, published 03/00.

¹ Reference [2], pp.10-11.

5. INTERAGENCY WORKSHOPS ON ADVANCED BATTERY TECHNOLOGIES

A. Workshop on Interfaces, Phenomena, and Nanostructures in Lithium Batteries

Ken Heitner

U.S. Department of Energy

EE-32, Room 50-030

Washington, DC 20585-0121

(202) 586-2341, fax: (202) 586-1600, e-mail: kenneth.heitner@ee.doe.gov

Albert Landgrebe

Consultant

(302) 945-4306, fax: (302) 945-2219, e-mail: albert@dmv.com

Objectives

- Assemble experts from industry, national laboratories, and academia to:
 - Review current research on interfaces, phenomena and nanostructures in lithium-ion and lithium polymer batteries for EV and HEV applications emphasizing both applied and basic studies.
 - Increase knowledge of the electrochemical interfaces that occur within electrodes and at the electrode/electrolyte interfaces and the applications of nanostructures in electrodes and electrolytes.
 - Continue interactions and information exchange between individuals concerned with research and those concerned with battery development.
 - Continue to improve collaboration and communication between academics and industry.

Approach

- Provide a critical review of the current status of our understanding of the chemistry, solid state physics, and engineering of relevance to lithium battery technologies for EV and HEV applications.
- The research includes:
 - interactions of cathode materials,
 - interactions of anode materials,
 - nanomaterials,
 - ion transport, and
 - characterization of interfacial phenomena.
- Identify problem areas and barriers to future progress in this field.

Accomplishments

- Thirty-seven papers and presentations on various areas of interest generated and published.

Future Directions

- A workshop on alternatives anodes, non-lithium, is being organized for August 2002.
-

Workshop Technical Synopsis

A workshop on Interfaces, Phenomena, and Nanostructures in lithium batteries was held December 11-13, 2000 at Argonne National Laboratory, Argonne, Illinois. The purpose of the workshop was to assemble experts from industry, laboratories, and academia to review current research on interfaces, phenomena and nanostructures in advanced batteries for EV and HEV applications. It emphasized both applied and basic studies.

Session 1. Overview

Mr. Duong described battery research [1] sponsored by the US DOE Office of Advanced Automotive technologies (OAAT). The main objective is to promote technology and scientific transfer between the projects at the DOE national laboratories and universities and the battery technology development projects sponsored by the United States Advanced Battery consortium (USABC).

Dr. Maupin reported on the current and past program priorities and history of Electrochemical Energy Storage and Conversion Program in the Office of Science's Basic Energy Sciences Program. The emphasis is on the need for increase fundamental understanding in electrochemical processes.

Dr. Carlin reported that a major focus of the basic research supported by the Office of Naval research is the utilization of nano-materials in electrochemical energy storage and conversion. He stated that nano-structured electrodes and electrolytes can enable unprecedented performance and may provide a means to break the classic Ragone paradigm of energy versus power.

Session 2. Status and Requirements

This session consisted of three presentations.

Dr. Newman [2] reported on the use of modeling as the roadmap to battery requirements. Such performance modeling is useful in predicting discharge curves, responses to driving profiles, including regenerative braking, and heat generation and heat transfer characteristics necessary for good thermal management. The models can help elucidate the material properties and how they affect battery performance.

Dr. Brodd [3] reported on the recent history of lithium-ion battery developments and reported on the commercial quantities of lithium-ion, lithium-polymer and lithium-ion polymer batteries.

Mr. Henriksen [4] gave a talk on test and diagnostic methods used to study interface phenomena in high-power lithium-ion cells. For the cells with $\text{LiNi}_{0.8}\text{Co}_{0.2}\text{O}_2$, the results indicate that surface and interface phenomena are the primary cause of power fade.

Session 3. Cathode Materials Interactions

The four papers in this session covered the causes and effects for the changes in the performance of manganese oxide cathode materials. Lithium manganese oxide (spinel or LMO) cathode materials have many positive attributes: low cost, high power density, excellent safety characteristics, and minimal bio-hazard risk. Stoichiometric spinel is susceptible to rapid deterioration during battery cycling and considerable effort has been expended to stabilize LMO. Two approaches are to coat the spinel particles with an acid-resistant species or replace a fraction of the Mn^{+3} with another cation.

A subset of this latter approach reported by Dr. Howard [5] is the use of excess Li to produce non-stoichiometric $\text{Li}_{1+x}\text{Mn}_2\text{O}_4$. He reported that small mean particle sizes are more difficult to handle but offers greater available capacity at high discharge rates, an important asset for automotive battery use.

Dr. Johnson [6] reported on the preparation and characterization of layer manganese oxide materials for use in electrodes in lithium batteries. An important discovery was that at high rate, small particle size may offer better capacity retention, one of the critical issues for automotive use.

Dr. Striebel [7] reported on the formation of the SEI layer on LiMn_2O_4 films. Nine parameters were investigated and the effects with state of charge and changes with cycling were determined.

Dr. Cairns [8] has made progress in elucidating the role of metal substitution in enhancing the cycle life of metal-substituted spinel. It was shown that the spinels are damaged by the presences of moisture in the electrolytes.

Session 4. Interactions of Anode Materials

Considerable activity has been directed at increasing the capacity (mAh/g) of anode materials. Hard carbons can exhibit higher capacity.

Mesophase pitch fibers are used in commercial cells. An overview of the wide variety of carbons available for negative electrodes in Li-ion batteries, and the electrochemical results obtained on graphite electrodes was reported by Dr. Kinoshita [9].

The search for higher capacity anode materials [10, 11, 12] has led investigators to revisiting the lithium alloy materials, especially lithium tin alloys. These materials have good high rate charge and discharge rates but poor cycle life at deep depths of discharge. The volume change on charge-discharge causes the alloy to break up with loss of contact with the current collector.

Dr. Thackeray described the use of inter-metallic electrodes that use a non-alloying element such as copper and iron to provide an inactive matrix that can absorb part of the dimensional changes that occur on cycling. Also, the electrochemical reactions of lithium with InSn are compared with those of metal oxides such as Fe_3O_4 .

Dr. Visco explained that Polyplus Battery company is involved in the development of reversible electrodes based on lithium metal. This is accomplished through the development of an engineered lithium electrode composed of lithium metal foil coated with ultra-thin (500-1000 Å) glass.

Dr. Reilly described the preparation and properties of Li nanocomposites [12] produced via hydrogen driven, solid state, metallurgical reactions.

Session 5. Nano-Materials

Nanoscience and nanotechnology-not so long ago only futuristic, speculative ideas- are now vibrant real areas of scientific research and engineering development. In this workshop, the application of nanotechnology to polymer electrolytes and template electrode materials were reported.

Dr. Hackney [13] is studying the multi-phase transformation in intermetallic compounds for Li-ion batteries. The present work is to provide a framework to examine nanostructural development within the context of classical phase transformation theory. The result is a predictive model of micro length scale and electrochemical properties.

Dr. Rolinson [14] reported on nanoscale, high surface area and highly porous MnO_2 that were prepared using sol-gel chemistry. The noncrystalline MnO_2 resulted in improved charge storage properties at high charge/ discharge rates.

Dr. Sadoway [15] studied the use of block copolymers in nanostructured architectures in lithium batteries. In charge/discharge tests hundreds of cycles at rates as high as 4C were obtained. These electrodes exhibited high resistant to capacity fade.

Dr. White [16] reported on transport phenomena at nanoscale dimensions. The preliminary results suggest that molecular transport of electro active species to electrodes of dimensions below 100 nm is significantly influenced by interfacial electric fields, resulting in the enhancement or diminishment of Faradaic currents.

Dr. Kostecki [17] reported on the use of contact AFM for nanoscale-scale electrochemical lithography of thin LiMnO_4 films.

Dr. Kumta [18] described the preparation of new nanostructured silicon-based composites that will be used as new electrode materials for lithium batteries. Nanocomposites containing various molar ratio of Si and TiN were fabricated. Electrochemical cycling shows no cracking and excellent phase retention suggesting the potential of these nanocomposites for use as lithium-ion cell anodes.

Dr. Patrissi [19] revealed two new methods that were used to increase the volumetric capacity of V_2O_5 electrodes. Membrane-based template synthesis was used to prepare nanostructured V_2O_5 electrodes.

Session 6. Ion Transport Relationships of Structure to Performance

Understanding electron and ion transport through electrode/electrolyte interfaces remains one of the principal challenged for continued progress in lithium battery development. For example, even within a single battery component such as a nano composite polymer electrolyte, there are many interfaces associated with the large surface area of the nano particle component.

Dr. Curtiss [20] carried out a theoretical study of lithium affinities of salts used in polymer electrolytes. The lithium affinities in kcal/mole were reported for several salts.

Dr. Grey [21] used ^6Li MAS NMR to study lithium manganese oxide materials. The introduction of defects or dopant cations into the structure results in an increase in manganese oxidation state near the defects. Lithium ions near the defects are, therefore, deintercalated at higher voltages than the lithium ions in the bulk.

Dr. Skandan [22] developed a new class of nanostructured materials for use in rechargeable lithium-ion and hybrid batteries. Unlike micro-sized powers, ultra fine $\text{Li}_4\text{Ti}_5\text{O}_{12}$ showed good retention capacity at a discharge rate as high as 10C in $\text{Li}/\text{Li}_4\text{Ti}_5\text{O}_{12}$ cells.

Session 7. Characterization of Interfacial Phenomena in Lithium-ion and Li-Polymer Batteries.

The term solid electrolyte interphase (SEI) denotes an identifiable material phase residing at the electrode/electrolyte boundary.

Dr. Yang [23] determined the structures and electrochemical performance of several cathode materials for lithium-ion batteries. In-situ studies of cathodes cycled at high rates were carried out. Several cathodic materials were examined by in-situ XAS and XRD and the changes in electrochemical performance were related to changes in structure.

Dr. Mukerjee [24] reported on the effect of Ni and Co substitution in Mn oxide spinel cathode electrodes. Partial substitution greatly affects the electrochemistry and cycle life of the cathode. In-situ XAS was used to determine the exact nature of the oxidation state changes in order to explain the overall capacities at the different voltage plateaus.

Dr. Kostecki [25] used SERS and atomic force microscopy to study interfacial phenomena on selected cathode materials. He identified detrimental processes which occurred at the electrode/electrolyte interface for thin-film LiMn_2O_4 electrodes. Temperature-induced surface degradation properties of $\text{LiNi}_{0.8}\text{Co}_{0.2}\text{O}_2$ cathode were also determined.

Dr. Amine [26] determined that for high power, 18650 lithium-ion cells that surface phenomena was responsible for the impedance rise.

Dr. Teeters [27] used self-assembled molecular layers (SAMs) to stabilize the lithium/polymer electrolyte interface.

Dr. Mansour [28] reported on the use of XAS and electrochemical characterization methods to follow the evolution of the oxidation state and atomic structure of Sn as a function of Li content during charge and discharge cycle of crystalline $\text{Sn}_2\text{P}_2\text{O}_7$.

Dr. Doeff [29] reported on manganese oxides with the $\text{Na}_{0.44}\text{MnO}_2$ that can undergo prolonged cycling with little or no capacity fade in the lithium

battery configurations at either room temperature or 85°C . There is no phase transition to the spinel.

Session 8. Polymer, Gel, and Composite Electrolytes

Dr. Halley [30] described the results on the dynamics of lithium ions in a molecular dynamics model of amorphous polyethylene oxide electrolyte and made suggestions for searching for more conductive polymer electrolytes.

Dr. Scanlon [31] described the use of computational chemistry to design a solid state ionically conducting channel for lithium ion.

Dr. Kerr [32] reported on the chemical, electrochemical and mechanical requirements for electrolytes at electrode interfaces. The nature of side reactions and the dynamic nature of the interface were reviewed.

References

- [1] J. Deppe, K. Heitner, T.Q. Duong,, P.H. Maupin, and A. Landgrebe, "Advanced Lithium Solid State Battery Developments," paper No. 2000-01-1588, the 2000 Future Car Congress, Arlington, VA, April 2000.
- [2] J. Newman, H. Hafezi, and C. Monroe, "The Roadmap to Battery Requirements", The Electrochemical Society Proceeding Volume 2000-36 (2000) 1-13.
- [3] R.J. Brodd, "Recent Advances in Lithium-ion Batteries", The Electrochemical Society Proceeding Volume 2000-36 (2000) 14-26.
- [4] G.L. Henriksen, "Test and Diagnostic Methods Used to Study Interface Phenomena in High-Power Lithium-ion Cells", The Electrochemical Society Proceeding Volume 2000-36 (2000) 27-35.
- [5] W.F. Howard, Jr., S.W. Sheargold, P.M. Story, and D. Zhang, "Performance Variations from $\text{Li}_{1+x}\text{Mn}_{2-x}\text{O}_4$ Cathode Materials: Cause and Effects", The Electrochemical Society Proceeding Volume 2000-36 (2000) 36-46.
- [6] C.S. Johnson and M.M. Thackeray, "Layered $(1-x)\text{Li}_2\text{MnO}_3 \cdot x\text{LiMO}_2$ (M=Ni, Co, Cr, or Mn) Electrodes for Lithium Batteries", The Electrochemical Society Proceeding Volume 2000-36 (2000) 47-60.
- [7] K. Striebel, E. Sakai, and E. Cairns, "Impedance Behavior of the $\text{LiMn}_2\text{O}_4/\text{LiPF}_6\text{-DMC-EC}$ Interface During Cycling", The

- Electrochemical Society Proceeding Volume 2000-36 (2000) 61-67.
- [8] M.C. Tucker, A. Braum, U. Bergmann, H. Wang, P. Glatzel, J.A. Reimer, S.P. Cramer and E. Cairns, “⁷Li MAS-NMR, X-ray Spectroscopy and Electrochemical Studies of LiMn₂O₄-Based Spinel for Lithium Rechargeable Batteries”, The Electrochemical Society Proceeding Volume 2000-36 (2000) 68-79.
- [9] K. Kinoshita, and K. Zaghbi, “Overview of Carbon Anodes for Lithium-ion Batteries”, The Electrochemical Society Proceeding Volume 2000-36 (2000) 80-91.
- [10] M.M. Tucker, J.T. Vaughey, C.S. Johnson, A.J. Kropf, H. Tostmann, R. Benedek, T. Sarankonsri, and S.A. Hackney, “Intermetallic Negative Electrodes for Lithium Batteries”, The Electrochemical Society Proceeding Volume 2000-36 (2000) 92-101.
- [11] D.A. Totir and D.A. Scherson, “In-situ X-ray Absorption Fine Structure and Raman Studies of Embedded Lithiated Manganese Oxide Particle Electrodes in Electrolyte Solutions of Relevance to Battery Applications”, The Electrochemical Society Proceeding Volume 2000-36 (2000) 102-113.
- [12] J.J. Reilly, J.R. Johnson, T. Vogt, G.D. Adzic, Y. Zhu, and J. McBreen, “Preparation and Properties of Li Nanocomposites Produced Via Hydrogen Driven, Solid State, Metallurgical Reactions”, The Electrochemical Society Proceeding Volume 2000-36 (2000) 114-133.
- [13] S.A. Hackney, “Multi-Phase Transformation in Intermetallic Compounds for Li-ion Batteries”, The Electrochemical Society Proceeding Volume 2000-36 (2000) 134-143.
- [14] J.W. Long, R.M. Stroud, K.E. Swider-Lyons, and D.R. Rolison, “Design Pore-Solid Architected in Nanostructured Battery Materials”, The Electrochemical Society Proceeding Volume 2000-36 (2000) 144-152.
- [15] A.M. Mayes, and D.R. Sadoway, “Using Block Copolymers in Nanostructured Architectures in Lithium Batteries”, The Electrochemical Society Proceeding Volume 2000-36 (2000) 153-162.
- [16] J.J. Watkins, B.D. Cope, J.L. Conyers, Jr., and H.S. White, “Transport Phenomena at Nanoscale Dimensions”, The Electrochemical Society Proceeding Volume 2000-36 (2000) 163-174.
- [17] R. Kostecki, X.Y. Song, K. Kinoshita, and F. McLarnon, “Nanoscale Fabrication and Modification of Selected Battery Materials”, The Electrochemical Society Proceeding Volume 2000-36 (2000) 175-184.
- [18] I.S. Kim, P.N. Kumta, and G.E. Blomgren, “Nanostructured Silicon Based Composites: New Anode Materials for Li-ion Batteries”, The Electrochemical Society Proceeding Volume 2000-36 (2000) 185-196.
- [19] J. Patrissi, and C.R. Martin, “Improving the Volumetric Lithium-Insertion Capacity of V₂O₅ Electrodes Prepared Using the Template Method”, The Electrochemical Society Proceeding Volume 2000-36 (2000) 208-222.
- [20] G. Baboul, and L.A. Curtiss, “Theoretical Study of Lithium Affinities of Salts Used in Polymer Electrolytes”, The Electrochemical Society Proceeding Volume 2000-36 (2000) 223-234.
- [21] Y.J. Lee, and C.P. Grey, “⁶Li MAS NMR Studies of Lithium Manganese Cathode Materials”, The Electrochemical Society Proceeding Volume 2000-36 (2000) 235-243.
- [22] A. Singhal, G. Skandan, G. Amatucci, and N. Pereira, “Nanostructured Electrode Materials for Rechargeable Li Batteries”, The Electrochemical Society Proceeding Volume 2000-36 (2000) 244-251.
- [23] J. McBreen, X.Q. Yang, M. Balasubramanian, and X. Sun, “Structural Characterization and Electrochemical Performance of Cathodes for Lithium-ion Batteries”, The Electrochemical Society Proceeding Volume 2000-36 (2000) 252-261.
- [24] S. Mukerjee, R.C. Urian, X.Q. Yang, J. McBreen, and Y.E. Eli, “Effect of Ni and Cu Substitution in Mn Oxide Spinel Cathodes for Electrochemical and In-Situ Synchrotron Spectroscopic Study”, The Electrochemical Society Proceeding Volume 2000-36 (2000) 262-271.
- [25] R. Kostecki, Y. Matsuo, and F. McLarnon, “Interfacial Phenomena on Selected Cathode Materials”, The Electrochemical Society Proceeding Volume 2000-36 (2000) 272-282.
- [26] K. Amine, J. Luo, C. Chen, A. Andersson, D. Vissers, “Surface Phenomena Responsible for Impedance Rise in Lithium-ion High Power

- Batteries”, The Electrochemical Society Proceeding Volume 2000-36 (2000) 283-287.
- [27] S. Gadad, and D. Teeters, “Characterization and Stabilization of Passivation at the Lithium/Polymer Electrolyte Interface: A Nanoscale Approach”, The Electrochemical Society Proceeding Volume 2000-36 (2000) 288-300.
- [28] A.N. Mansour, and S. Mukerjee, “X-ray Absorption and Electrochemical Studies of Tin-Based Oxide Electrodes”, The Electrochemical Society Proceeding Volume 2000-36 (2000) 301-308.
- [29] M.M. Doeff, T.J. Richardson, K.T. Hwang, A. Anapolsky, M. Gonzales, and L.C. DeJonghe, “Novel Tunnel-Containing Manganese Oxides with Excellent Reversibility”, The Electrochemical Society Proceeding Volume 2000-36 (2000) 309-316.
- [30] J.W. Halley, and Y. Duan, “Mechanisms of Lithium Conductance in PEO from Molecular Simulation”, The Electrochemical Society Proceeding Volume 2000-36 (2000) 317-325.
- [31] L.G. Scanlon, L.R. Lucente, W.A. Feld, G. Sandi, D.J. Campo, A.E. Turner, C.S. Johnson, and R.A. Marsh, “Lithium-ion Conducting Channel”, The Electrochemical Society Proceeding Volume 2000-36 (2000) 326-339.
- [32] Y.B. Han, J. Hou, J.B. Kerr, K. Kinoshita, J.K. Pugh, C. Leiva-Parades, S.E. Sloop, and S. Wang, “Chemical, Electrochemical, and Mechanical Requirements for Electrolytes at Electrode Interfaces”, The Electrochemical Society Proceeding Volume 2000-36 (2000) 340-352.

B. Workshop on Development of Advanced Battery Engineering Models

Ken Heitner

U.S. Department of Energy

EE-32, Room 50-030

Washington, DC 20585-0121

(202) 586-2341, fax: (202) 586-1600, e-mail: kenneth.heitner@ee.doe.gov

Albert Landgrebe

Consultant

(302) 945-4306, fax: (302) 945-2219, e-mail: albert@dmv.com

Irwin Weinstock

Sentech, Inc

(301) 654-7224, fax: (301) 654-7832, e-mail: iweinstock@sentech.org

Objectives

- Assemble experts from industry, national laboratories, and academia to:
 - Review current research on advanced battery models for HEV and EV applications, emphasizing both applied and basic studies.
 - Increase awareness of vehicle systems analysis using DOE-supported advanced vehicle simulation tools such as ADVISOR and PSAT.
 - Increase interactions and information exchange between individuals concerned with battery modeling and development and those concerned with applying batteries as power sources in HEVs and EVs.
 - Continue to improve collaboration and communication between academia and industry.

Approach

- Provide a critical review of the current status of vehicle simulation models and battery models.
- Identify factors that limit the functioning of battery performance, failure, and thermal models and of vehicle simulation models (ADVISOR and PSAT) that are not being met by current modeling efforts. Make recommendations to DOE for specific areas of research that would overcome such limiting factors.
- Identify problem areas and barriers to future progress in this field.

Accomplishments

- The workshop involved more than 60 participants from the automobile industry, battery manufacturers, academic institutions, national laboratories, the DOE, and other government agencies. The participants heard presentations and panel discussions on various areas of interest to vehicle and battery modelers and took part in open forums that addressed the questions of what additional work is needed to enhance the capabilities of battery and vehicle simulation models and how the data needs of the developers and modelers can be addressed.

Future Directions

- A symposium entitled, "Power Source Modeling" has been organized for the 202nd Meeting of the Electrochemical Society in Salt Lake City, UT, October 20–25, 2002.
-

Workshop Technical Synopsis

A workshop on the Development of Advanced Battery Engineering Models was held August 14–16, 2001, at Doubletree-Crystal City Hotel in Arlington, VA. The purpose of the workshop was to review current research on advanced battery models for HEV and EV applications, emphasizing both applied and basic studies, increase awareness of vehicle systems analysis using DOE-supported advanced vehicle simulation tools such as ADVISOR and PSAT, increase interactions and information exchange between individuals concerned with battery modeling and development and those concerned with packing and applying batteries as power sources in HEVs and EVs, and continue to improve collaboration and communication between academics and industry. The presentations from this workshop are summarized in its Proceedings [1] and detailed papers will be included in a forthcoming special issue of the Journal of Power Sources [2].

Opening Session

Dr. Raymond A. Sutula opened the workshop by presenting an overview of the current status and plans for HEV and EV applications. He reported that a goal of the Energy Management and Vehicle Systems Teams is to develop and validate models and simulation programs that are useful for predicting fuel economy and emissions and aid in setting performance targets for electric and hybrid vehicles.

Dr. Kenneth Heitner described battery research sponsored by DOE's Office of Advanced Automotive Technologies (OAAT). The main objective of its R&D effort is to promote technology and scientific transfer between the projects at the DOE national laboratories and universities and the battery technology development projects sponsored by the United States Advanced Battery Consortium (USABC) and the Partnership for a New Generation of Vehicles (PNGV).

Session 1. Vehicle and Power System Simulation Models

Dr. Tony Markel described hybrid vehicle system analysis and optimization using the ADVISOR simulation model developed at NREL. The evaluation methodology, assumptions, basic

components and fuel economy results were reviewed. A demonstration illustrated the capability of the model to optimize a hybrid system based on multiple components and control strategies.

Dr. Aymeric Rousseau described the PSAT model and the Advanced Powertrain Test Facility at Argonne National Laboratory. The PSAT architecture is designed to facilitate development of control algorithms for drivetrains and vehicle system optimization. The test facility is used for model validation, validation of components and subsystems, benchmarking of new technologies, and development of test procedures.

Dr. Roger Dougal discussed the virtual test bed for advanced battery systems developed at the University of South Carolina. The model has been applied to lithium-ion and nickel-metal hydride batteries. The model includes an improved method of treating thermal effects in batteries.

Session 2a. Battery Performance Models

Dr Vincent Battaglia presented a summary of the remarks prepared by Dr. John Newman. The presentation showed how battery modeling can promote our understanding of processes, identify critical parameters and materials' properties, permit optimization relative to design goals, allow us to approach failure mechanisms, and provide a context for invention and characterization of materials.

Dr. Roger Dougal reported on the progress of battery performance modeling at the University of South Carolina. Key factors identified for maximizing the specific power of a cell are: utilizing cells with high OCV, minimizing over potentials, reducing the weight and volume of cell components, and utilizing thinner cells and separators. Future tasks include validation of a 3D stack model, detailed study of the effects of pulse charge/discharge and capacity effects, and development of a more detailed thermal/electrochemical model.

Dr. Bor Yann Liaw reported on the integrated advanced battery R&D simulation and modeling development being carried out at the University of Hawaii. His presentation indicated that advanced modeling and simulation with detailed validation is a powerful tool for battery development. In-depth understanding of battery performance is the key to successful vehicle applications, and combining

simulation and experimental analysis facilitates system integration.

Dr. Dees gave a brief discussion on transport measurements for lithium ion conducting polymer electrolytes. An engineering model approach was used to obtain a complete set of transport and thermodynamic properties for a binary salt dissolved in a polymer electrolyte. The technique was based on concentrated solution theory and required a minimal amount of experimentation. Results from measurements on a representative polymer electrolyte system were given. The measured transport and thermodynamic properties of the polymer electrolyte were used to simulate the performance of symmetric Li/polymer/Li cells.

Dr. Johnson described the various battery models available within the ADVISOR vehicle simulation program. These include three equivalent circuit models of increasing complexity: a fairly simple internal resistance model based on available battery data, a resistance-capacitance equivalent circuit model derived from SAFT's two-cap model, and an equivalent circuit model based on the PNGV battery test manual which is currently undergoing validation. ADVISOR also contains a neural network model and a fundamental phenomenological model for lead acid batteries.

Luncheon Speaker

Dr. Verbrugge's talk was entitled, "From mathematical modeling of batteries to vehicle integration of batteries." The discourse covered modeling of high power density carbon electrodes for lithium ion batteries, transitioning from relatively fundamental models to vehicle integration, and a simple model that has been used in GM vehicle integration programs.

Session 2b. Battery Performance and Economic Models

Dr. Sack reported on the Energy Balance model developed at SAFT for lithium-ion cells. The model assumes that the energy stored in the battery can be determined by integrating the power flows into and out of the cells and the losses inside the battery. It can be expanded from the cell level to the battery level as required. Input driving profiles can be based on power, energy per unit of time, or current. Dynamic thermal effects are included so that

changes in impedance are reflected in the predictive performance.

Dr. Wright reported on elevated temperature calendar and life test studies of advanced technology development program generation one lithium ion batteries. The test data reported agreed with that reported in the literature. An empirical equation describing the nonlinear increase of cell resistance with time at elevated temperatures was developed.

Dr. Paez described the techniques used in inductive modeling of lithium ion cells, including singular value decomposition and artificial neural networks. Applications of inductive modeling to lithium ion cells and other batteries were presented. When these models were applied appropriately they resulted in accurate characterization of the battery behavior.

Dr. Nelson has designed a model that has been applied to PNGV applications. The model has been successfully used to calculate the weight, volume, power, available energy and operating voltage range of lithium ion batteries. This allows cells and batteries with various form factors and thermal management systems to be designed to meet PNGV criteria.

Dr. Gaines presented results of lithium-ion EV and HEV battery cost studies. Areas where research could reduce costs were identified.

Session 3. Battery Thermal Models

Dr. Pesaran explained the thermal modeling efforts currently underway at NREL, including the types of data and error limits that are needed for the ADVISOR thermal model. There is a need to obtain experimental data so ADVISOR can be used to transfer laboratory information into vehicle control methodology.

Dr. Al-Hallaj described a thermal management system for EV batteries using phase change materials (PCM). Simulation using commercial software showed that the PCM system could improve the performance of the Sony ALTRA-EV™ Battery by keeping the battery at a uniform and elevated temperature during discharge and relaxation.

Dr. Doughty described Sandia National Laboratory's efforts to develop a thermal experimental and modeling project. Major emphasis is on acquiring data that can be utilized in thermal models. Other important considerations are the

effects of electrode, cell and battery structures on safety.

Dr. Wang provided an overview of the capabilities of his model in describing the thermal behavior of Li-ion cells. The emphasis is on understanding the underlying phenomena during operation. Case studies were reported that illustrate the importance of cooling, especially for cells in a stack. The model can explore the SOC imbalance between the different cells in the stack, which can lead to a thermal excursion. The effects of these imbalances and the methodologies for addressing them were explained.

Dr. Nelson reported on modeling of thermal management for Li-ion PNGV batteries, including design of a liquid-based thermal management system and sufficient insulation to prevent high temperatures when the battery is in standby conditions.

Session 4. Fundamental Physical Phenomena in Model Development

Dr. Landgrebe introduced the topic by explaining that the development of batteries spans several orders of magnitude in time, from molecular processes that occur in pico seconds to driving profiles that occur over several hours, as well as in size, from the molecular scale to the dimensions of full-sized EV battery packs. This is illustrated graphically (Figure 1).

Dr. Blomgren described the processes leading to formation of a film on the electrode surface during the first cycle of a lithium ion cell. This is called the solid electrolyte interphase (SEI) layer. The composition of the film depends largely on the makeup of the electrolyte. The beneficial effects of additives to electrolytes to improve low temperature performance were also reported.

Dr. Halley described his efforts to model lithium ion conduction in polyethylene oxide (PEO). Mechanisms of lithium ion conduction in PEO were determined using a molecular simulation model of the dynamics of lithium ions in PEO. This modeling has led to an understanding of how to make better polymers.

Dr. Kerr from LBNL reported that the future of ambient temperature lithium-polymer batteries may depend upon the development of new polymer materials that possess novel, kinetically labile solvating groups, allow a decrease in separator

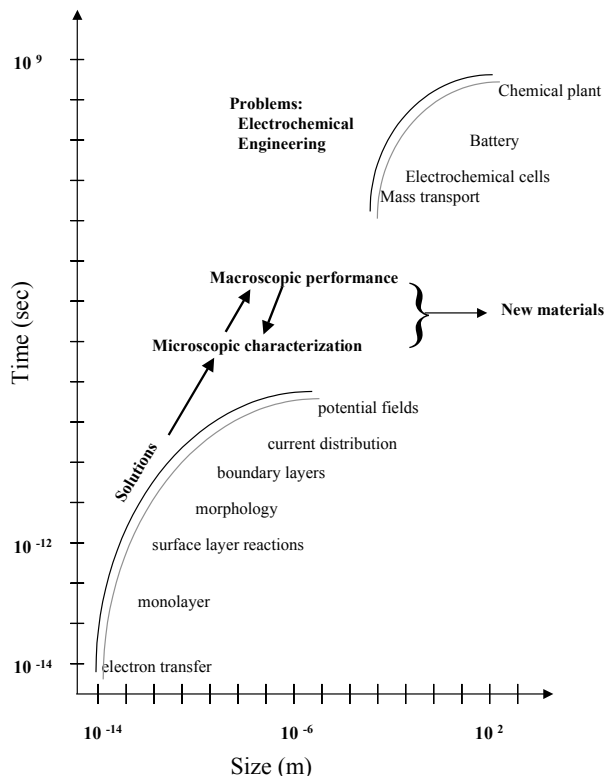


Figure 1. Battery Development Timeframe

thickness, operate with added solvent, or contain immobilized anions to yield polyelectrolytes with unity transference numbers and sufficient conductivity to produce a useful battery.

Dr. Kinoshita presented an overview of the strides made in carbon anode technology. The best results were yielded by hard carbons at 650 mAh/g with 85% efficiency and graphites at 450 mAh/g with 92% efficiency. Analysis of alternative anode materials and summary physicochemical parameters and electrochemical parameters for Li-ion batteries that are useful in modeling were presented.

Dr. Cairns reported on studies conducted at LBNL on lithium alloy and Mg₂Si thin film anodes for secondary lithium batteries. Possible improvements might involve the ability to operate safely at higher current densities, less first cycle irreversible capacity loss, better cycling behavior, reduced volume and lower cost. One of the problems with metal-metal alloys is decrepitation due to large volume changes, which results in capacity losses upon cycling. A model to explain failure mechanisms is being developed.

Dr. Thackeray described work on synthesizing and characterizing intermetallic anode materials for

lithium batteries. The primary focus has been on finding materials with a strong relationship between parent and lithiated structures in an attempt to create a stable host framework for lithium intercalation/deintercalation.

Dr. Benedek reported on modeling lithium reactions with intermetallic compound electrodes. The nature of the volume expansion caused by lithium intercalation via interstitial diffusion for selected antimonides, stannides and silicides was reported.

Dr. Curtiss reported on quantum chemical studies of lithium electrolytes. The objective was to improve the performance of the electrolyte by obtaining a fundamental understanding of ion-association processes and ion polymer interactions and the role they play in ionic conductivity in lithium polymer batteries. Electronic structure calculations, molecular dynamics simulations and experimental studies using neutron diffraction and NMR have been carried out. Binding energies were determined and redox potentials and reaction mechanisms were calculated.

Dr. Garofalini applied the molecular dynamics computer simulation technique to studies of thin film lithium ion batteries and has shown results that are consistent with the structural features of the cathode crystal and the electrolyte glass films. The simulations illustrated the effects of interfacial bonding on phase transformation in the glass and the impact of diffusion anisotropy on lithium migration into the crystal. The results also indicate that the relaxation of the ions in the metasilicate glass enables a smoothing of rough interfaces.

Session 5. Data Needs and Sources

Panelists, including Chester Motlock, Scott Jones, Matthew Keyser, and Ivan Menjak each presented a short overview of the testing procedures and data analysis techniques employed in their respective laboratories. This was followed by an active discussion among all the participants on issues related to collecting, corroborating, and disseminating battery data.

Session 6. Model Outputs-Industry Perspectives.

A panel made up of representatives from DaimlerChrysler, Ford, General Motors, and Delphi

Automotive presented the auto industry perspectives on battery modeling.

The panelists presented the automakers' requirements for battery models and described the characteristics of the ideal battery model. Battery performance and thermal model requirements were defined in terms of minimum and desired outputs. Model verification was discussed and recommended variables offered. Other complimentary data needs were also mentioned.

Wrap-up

The workshop wrapped up with two open forums in which the participants discussed issues related to data gathering and dissemination and to the future course of DOE-supported battery modeling activities.

During these sessions, the participants were reminded of the large amount of modeling capability that is in place, working to develop models from the vehicle system level down to the component levels. DOE-sponsored vehicle-level modeling activities are focused at two national labs, NREL and ANL, supported by additional work at INEEL and SNL. A third vehicle-level modeling team is in place, headed by the University of South Carolina.

Battery-level modeling efforts covering electrical performance, thermal responses, and economics are also underway at several national labs and universities. DOE-sponsored research also supports the development of molecular development of molecular-level models that describe fundamental physical phenomena occurring in batteries, such as the transport of ions in polymer electrolytes.

The workshop participants concluded that engineering models for advanced battery technologies need to be standardized to meet the industry's needs. Formats for collecting and reporting battery data used in developing, validating, and exercising these models should also be standardized to facilitate data exchange among various investigators. A means should also be found to expedite testing at the national laboratories and to facilitate wider dissemination of the test results.

It was also recommended that the national labs should focus on developing open versions of the models that are compatible with the industry's needs and current practices. These open models should be validated for commonly available battery

technologies that can be obtained by the labs and used as calibration items.

Development of component-level models that are primarily research and development tools should also be strengthened. This could be an on-going responsibility of the Batteries for Advanced Transportation Technologies (BATT) Program. An effort should be made to increase the synergy between the molecular model development and the search for improved electrolytes and electrodes.

References

- [1] Proceedings of the Workshop on Development of Advanced Battery Engineering, Arlington, VA, August 2001.
- [2] Journal of Power Sources, Special Issue on Engineering Modeling of Lithium Batteries, In press.

6. ADVANCED BATTERY READINESS GROUP

A. Advanced Battery Readiness Ad Hoc Working Group (ABRWG) Meeting

Ken Heitner

U.S. Department of Energy

EE-32, Room 50-030

Washington, DC 20585-0121

(202) 586-2341, fax: (202) 586-1600, e-mail: kenneth.heitner@ee.doe.gov

Carol J. Hammel

National Renewable Energy Laboratory

(202) 646-5052, fax: (202) 646-7780, e-mail: carol_hammel@nrel.gov

Objectives

- Assess environmental and safety issues associated with advanced batteries for electric and hybrid electric vehicles.

Approach

- Form and coordinate government-industry partnerships to address the regulatory issues associated with introducing electric and hybrid electric vehicles, and their battery systems to the marketplace.
- The areas includes:
 - Shipping issues,
 - recycling/reclamation issues, and
 - in-vehicle safety issues.
- Identify problem areas and barriers to future progress in this field.

Accomplishments

- An ABRWG meeting was held in Washington, D.C., on February 28 - March 1, 2001.

Future Directions

- Continue with working group activities, as planned during the ABRWG meeting.

Introduction

An analysis of the environmental and safety issues for any new technology is an important part of the commercialization of that technology. This is particularly true of transportation-based technologies, such as electric and hybrid electric vehicles (EVs and HEVs). Safety is a critical factor for consumer acceptance. Environmental issues associated with battery systems, such as end-of-life recycling, and the safe shipment of batteries

containing hazardous materials, are also important factors in successful commercialization.

Meeting government regulations is a corollary issue as new technologies are introduced. When considering EVs and HEVs, the U.S. Department of Transportation (DOT) and the U.S. Environmental Protection Agency (EPA) play a key role in determining which aspects of the advanced vehicle system are regulated. DOT regulates both in-vehicle safety and hazardous materials shipping through the National Highway Traffic Safety Administration (NHTSA) and the Research and Special Programs

Administration, respectively. Because the EPA regulates solid and hazardous waste, it is responsible for determining parameters for recycling and reclamation of battery waste.

DOE has been working to address infrastructure barriers to the commercial acceptance of EVs and HEVs since the early 1990s. As an outgrowth of a workshop held in early 1990 on sodium beta batteries, a working group was established to identify and recommend solutions to barriers in the areas of battery shipping, battery reclamation/recycling, and in-vehicle safety. The Advanced Battery Readiness Ad Hoc Working Group, as it is now known, continues to provide a forum for discussion of these issues. The Working Group is composed of governmental officials, private-sector representatives from battery and automotive companies, recycling and chemical-processing companies, and representatives from the electric power partnerships such as the Electric Power Research Institute. Since its formulation in 1991, the Working Group has collectively considered a multitude of issues on sodium-beta, nickel /metal hydride, lithium-ion, and lithium-polymer batteries. In addition, safety issues relating to advanced vehicles have been extensively reviewed.

ABRWG Meeting, 2001

The Advanced Battery Readiness Ad Hoc Working Group (ABRWG) met at the Hyatt Arlington Hotel in Washington, D.C., on February 28 - March 1, 2001.

General Session Program

At the beginning of the general session, in his address entitled "U.S. DOE Program Overview and Directions", Ken Heitner of DOE discussed the January 25th decision by the California Air Resources Board (CARB) concerning the Zero Emissions Vehicle (ZEV) Program. He then discussed a status of commercial introduction of HEV and EV batteries and ongoing developments by Japan Storage Battery and Shin-Kobe, and the impact of CARB. It is projected that the number of hybrids sold will be 50,000 by 2004 and 250,000 by 2008 and the number of EVs would reach 50,000 in 2008. Shipping issues are nearly all resolved. In the in-vehicle safety area, Society of Automotive Engineers (SAE) has generated a number of recommended practices regarding how to build

hybrids and EVs, as well as the associated battery system in an acceptable manner. This assures a high level of abuse tolerance (SAE Recommended Practice J2464). A USABC report about abuse testing is also widely available. National Highway Transportation Safety Administration (NHTSA) has completed rulemaking on FMVSS Safety Standard #305, based on SAE J1766 (Battery Systems Integrity Crash Testing). Underwriters Laboratories (UL), National Fire Protection Association (NFPA), and International Standard Organization (ISO) have also defined appropriate standards for EV and HEV vehicle charging systems. The Infrastructure Working Council (IWC) has played a significant role in defining the infrastructure and its associated standards. International and domestic coordination between these standards setting organizations continues. Both conductive and inductive charging systems work safely.

In the reclamation and recycling arena, the takeoff curve for advanced batteries is getting well defined. The number of vehicle batteries available for recycling or reclamation could become the dominant factor in the recycling considerations.

Dr. Fritz Kalhammer, a consultant in electrochemical energy and process technology, reviewed the theoretical maximum specific energies of various battery systems, compared to the near term and longer term USABC criteria. He also reviewed the status of nickel metal hydride, lithium ion, lithium polymer EV batteries, and hybrid electric vehicle (HEV) batteries. Table 1 contains a summary of this status, along with his suggestions.

In his address entitled "Battery Collection and Recycling in Japan", Dr. Noboru Arai, Managing Director, LIBES, Japan, discussed battery sales and collection statistics, regulations, collection and recycling systems, examples of recycling process, and future issues. The Japan "Recycling Law" (Law for Promoting the Utilization of Recyclable Resources) was enacted in 1991. It is expected to be amended during 2001 and will cover Ni-Cd, Ni-MH, Li-ion, sealed lead acid batteries as 2nd category products. Future issues include: 1) how to promote collection by expanding the collection points and routes, engaging in public information and education, and aiming at batteries hoarded by consumers. 2) improving and developing recycling technologies for advanced batteries and reduce cost of recycling. 3) promote economical concentrated

treatment to cover different battery components and materials.

Mr. Frits Wybenga, Deputy Associate Administrator for Hazardous Materials Safety, Research and Special Programs Administration, U.S. Department of Transportation, in his presentation entitled "U.N. Process to Update Lithium Battery Shipping Requirements", discussed the international bodies and regulatory authorities on the transport of dangerous goods. The UN Manual provides the classification criteria for dangerous goods such as explosives, flammable solids, oxidizing materials, etc. It also provides the testing requirements for lithium batteries in Section 38.3. He explained the process through which UN recommendations are

incorporated into other standards and requirements as well as the history of the lithium battery requirements.

Mr. Michael E. Wilson, Manager, Governmental and Industry Relations, for Automotive Recyclers Association (ARA) provided a brief description of the activities of ARA, which has 1300 members in 14 countries. The industry supplies crash replacement parts and promotes reuse of recycled parts. In the U.S., the vehicle mercury switch disposal issue is related to the ELV recycling issue. ARA believes that automakers responsible for the creation such switches should also be responsible for their disposal. Mr. Wilson described the Certified Automotive Recycler (CAR) program established by the ARA to train and certify recyclers to ensure additional steps are taken to ensure environmental compliance and encourage the best business practices.

Table 1. Requirements and Goals for EV Batteries

Battery Characteristics	USABC		Suggested
	Mid-term	Long-term	
Requirements			
Electric range (miles)	~100	~150	~150 (200 ^b)
Weight (kg)	250 ^a	150 ^a	150
Capacity (kWh)	20 ^a	30 ^a	25
Power (kW)	30 - 40 ^a	60 ^a	50
Life (years)	>=5	>=10	>=10
Cost (\$)	~3000 ^a	~3000 ^a	~5000 ^a
Goals			
Specific Energy (Wh/kg)	>=80 to 100	>=200	>=150
Peak Specific Power (W/kg)	>=150	>=400	>=300
Cycle Life (80% DoD)	>=600	>=1000	>=1000 (>=500, 5-yr.)
Specific Cost (\$/kWh)	=<150	=<100	=<150 (= <200)
- For 5-year battery			
- For 10-year battery			
Battery life cycle cost (approximate) (¢/mile)	~6.3 ^a	~4 ^a	~6.3 ^a (5.2 ^{b,c})

Notes:

^a Inferred from battery life and cost goals

^b for high-efficiency, lighter-weight EV delivering 6-7 miles per kWh

^c assuming battery life determined by life cycle.

Briefing on Subworking Group Agendas

Gary Henriksen, Chair, Shipping Subworking Group presented a status summary of existing domestic and world shipping regulations for mid-term batteries such as sodium-beta and Ni-MH and long-term batteries of Li-ion and Li-polymer. He reviewed the amended UN documents published in mid-1999 and the Shipping Subworking Group (SSWG) activities in 2000. He reported on the SSWG contributions to the actions of the UN Committee of Experts in December 2000 and key amendments to UN 3090.

Rudy Jungst, Chair, Recycling/Reclamation Subworking Group, discussed the goal of the Recycling/Reclamation Subworking Group (RRSWG) and the major issues in the recycling of lithium-ion, lithium-polymer, and NiMH batteries, including regulatory changes. He then presented follow-up to the status of 2000 Action Items. Finally, the Battery Reclamation/Recycle Sub-Working Group agenda for this meeting was presented.

George Cole, Chair, In-Vehicle Safety Sub-Working Group, discussed the focus of the In-Vehicle Safety Sub-Working Group activities. He then summarized the group's recent accomplishments, a follow-up on 2000 Action Items and agenda for In-Vehicle Safety Sub-Working Group discussions.

Agenda Items

Shipping Subworking Group

- UN Actions at the December 2000 Meeting of the UNCOE
- Regulatory Activities Related to UN Amendments Incorporating “Large” Lithium Cells and Batteries

Recycling/Reclamation Subworking Group

- California ZEV Program Update
- Advanced Rechargeable Battery Recycling in Japan
- Sony Li-ion Battery Recycling in the U.S.
- Recovery and Recycling of Lithium Salts
- Status of Ni-MH EV and HEV Battery
- Recycling Update Study
- Update on Nickel and Cobalt Markets
- EV Battery Second Use Project
- EV Population Projections
- Regulatory Developments
- Future Directions

In-Vehicle Safety Subworking Group

- FMVSS 305 Update
- DOT Special Crash Investigations
- Hybrid-Electric Vehicle Battery Abuse Tests
- Battery In-Vehicle Safety Database
- Activities in Standards-making Organizations
- Emergency Responder Training

Future Action Items

Shipping Subworking Group

- Solicit information from DOE’s industrial lithium battery developers on the gross mass of their battery shipping units. The SSWG will use these to develop a gross mass limit on the packages that would contain these batteries and petition ICAO to increase the 35 kg/package mass limit that their provisions currently incorporate for the transport of lithium cells and batteries by cargo aircraft.
- Evaluate the size at which it is no longer practical to employ Group II packaging requirements and work through the USDOT to propose an amendment to UN Packing Instruction P903 that would allow for the

transport of properly encased lithium battery modules or battery units without the need for Group II packaging.

- Work through the USDOT to propose a new special provision to the UN Recommendations that would allow the transport of HEVs that incorporate “wet” batteries, “sodium beta” batteries, and “lithium” batteries.
- Work through one of the U.S. auto companies, or an umbrella organization like USCAR, to request a general exemption from USDOT to allow the transport of battery powered vehicles that incorporate lithium batteries to make the USDOT regulations consistent with the provisions of UN 3171.
- Work through one of the U.S. auto companies, or an umbrella organization like USCAR, to request a general exemption from USDOT to allow the transport of HEVs with large batteries (including “large” lithium batteries).
- Work with USDOT to ensure that their amended regulations conform to the amended UN Recommendations, per action items 2 and 3 at the international level.

Recycling/Reclamation Subworking Group

- Continue to watch progress of California ZEV program.
- Obtain information from other States on ZEV program plans.
- Invite Avestor to present information on Li-polymer battery recycling process development at next year’s meeting.
- Continue efforts to obtain information on rare earth recycling and on recovery of other metals such as vanadium from Ni/MH batteries.
- Attempt to find current information on the SNAM processing methods for Ni/MH batteries.
- Look at final results from the NREL study on Ni/MH battery recycling.

In-Vehicle Safety Subworking Group

- Follow up with an updated Emergency Responder Training course.
- Disseminate information collected during the follow-up to the participants via email as the effort progresses.

APPENDIX: ABBREVIATIONS, ACRONYMS, AND INITIALISMS

ABRWG	Advanced Battery Readiness Working Group
ANL	Argonne National Laboratory
CARB	California Air Resources Board
CPE	Composite polymer electrolyte
DOE	Department of Energy
DOT	Department of Transportation
EADL	Electrochemical Analysis and Diagnostics Laboratory (at ANL)
EC	electrochemical cell
EPA	Environmental Protection Administration
EV	Electric Vehicle
FY	Fiscal Year
HE	High Energy
HEV	Hybrid Electric Vehicle
HP	High Power
ISO	International Standard Organization
IVSSWG	In-Vehicle Safety Subworking Group
IWC	Infrastructure Working Council ()
LIBES	Lithium Battery Energy Storage Research Association of Japan
LIPON	Li Phosphorous Oxynitride
LMO	Lithium manganese oxide
NiMH	Nickel metal hydride
NHTSA	National Highway Traffic Safety Administration
NFPA	National Fire Protection Association
OAAT	Office of Advanced Automotive Technologies
OTT	Office of Transportation Technologies
PEO	polyethylene oxide
PNGV	Partnership for a New Generation of Vehicle
R&D	Research and Development
RPT	reference performance tests
SAE	Society of Automotive Engineers
SEI	Solid Electrolyte Interphase
SSWG	Shipping Subworking Group
UL	Underwriters Laboratories
UN	United Nations
USABC	United States Advanced Battery Consortium
ZEV	Zero emission vehicles

This document highlights work sponsored by agencies of the U.S. Government. Neither the U.S. Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the U.S. Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the U.S. Government or any agency thereof.

Office of Transportation Technologies Series of 2001 Annual Progress Reports

- Office of Advanced Automotive Technologies FY 2001 Program Highlights
- Vehicle Propulsion and Ancillary Subsystems
- Automotive Lightweighting Materials
- Automotive Propulsion Materials
- Fuels for Advanced CIDI Engines and Fuel Cells
- Spark Ignition, Direct Injection Engine R&D
- Combustion and Emission Control for Advanced CIDI Engines
- Fuel Cells for Transportation
- Advanced Technology Development (High-Power Battery)
- Batteries for Advanced Transportation Technologies (High-Energy Battery)
- Vehicle Power Electronics and Electric Machines
- Vehicle High-Power Energy Storage
- Electric Vehicle Batteries R&D



www.carttech.doe.gov

DOE/EERE/OTT/OAAT - 2001/013