New hydride-forming materials: challenges towards a new generation of high energy density Nickel-Metal-Hydride batteries

A. Ledovskikh[1], D. Danilov[2], A. Ayeb[1], and P.H.L. Notten[1,3,*]

[1] *Eindhoven University of Technology, Den Dolech 2, 5600 MB Eindhoven, the Netherlands*

[2] *Eurandom, Den Dolech 2, 5600 MB Eindhoven, The Netherlands*

[3] *Philips Research Laboratories, Prof. Holstlaan 4, 5656 AA Eindhoven, the Netherlands*

The new mathematical model to estimate volumetric and gravimetric energy densities of the rechargeable NiMH batteries has been proposed. Application of the new prospective $Mg_{0.80}Sc_{0.20}$ (1740 mAh/g) hydride forming material for MH electrode has been studied with the help of that model. It was shown that application of the new $Mg_{0.80}Sc_{0.20}$ material gives 58 % advance in gravimetric energy density (Wh/kg) for AA-size battery those expected capacity reaches 3045 mAh. For the battery having the same weight as normal AA-size battery higher gains have been achieved, namely, 5 % increase in volumetric energy density and 80 % in gravimetric. Thus prospective NiMH battery may compete with majority of the currently available lithium-ion batteries. The new binary (*e.g.* Mg-Ti) and ternary (*e.g.* Mg-Ti-Al) alloys having the same capacity as MgSc alloys can be implemented on a large industrial scale instead of expensive MgSc materials.

* To whom correspondence should be addressed (Peter.Notten@Philips.com)

1. **Introduction**

Clean, renewable and efficient energy storage became very important for our modern society. It facilitates sustainable development and provides environmental protection. In this respect, hydrogen is one of the most promising alternatives. Various techniques are available to store hydrogen, *i.e.* high-pressure, cryogenic and solid-state storages. The former two methods suffer from low weight efficiency. Moreover, the cryogenic storage requires a lot of energy to obtain and maintain the necessary storage conditions. Solid-state hydrogen storage, in the form of a metal hydride (MH) is typically characterized by high volumetric capacities. This is especially important for mobile applications because of space limitations. Nowadays, MH materials are used in high energy density Nickel Metal Hydride (NiMH) batteries, which are widely applied in many portable electronic devices and Hybrid Electrical Vehicles (HEV). [1-5].

Hydrogen is important also as energy carrier, because the traditional energy carriers, such as oil or gas will exhaust in the near future. In the transportation sector the consumption of fossil fuels can be reduced significantly by combining NiMH batteries with an internal combustion engine. Moreover, HEVs are ecologically cleaner than traditional cars. The expected sales growth of HEVs in the US is shown in Fig.1 (see [6]). It is apparent that number of HEVs is expected to increase significantly in the near future.

Commercially used MH ($LaNi_5$-based) compounds can typically store up to 1.2 wt% of hydrogen. Note that US Department of Energy has set a target for the weight efficieincy in year 2010 to 6 wt%. Thus, the gravimetric capacity of $LaNi_5$-based alloys is too low [7]. Therefore, a lot of research efforts had been made in the last years to increase the reversible hydrogen storage capacity. Recently, a breakthrough had been accomplished in the development of the new lightweight hydrogen storage materials. New Magnesium-Scandium alloy with a density of approximately $2 \cdot 10^6$ g/m^3 was developed by the group of Prof. Dr. P.H.L. Notten in the 'Portable Energy' laboratory of Philips NATLab. Experiments showed an incredible increase of the reversible storage capacity up to 6.7 wt% of H (see [7,8]). Fig. 2 illustrates increase in capacity of MgSc alloy in comparison with classical $LaNi_5$-based one. Apparently the capacity of new alloy even exceeds the requirements of the US Department of Energy. The Mg-Sc alloy is

characterized by a relatively low working pressure and can be efficiently applied for hydrogen storage via the gas phase. Fast kinetics of hydrogen absorption makes it possible to use this material in fuel cells and batteries.

NiMH batteries are nowadays successfully applied in the field of consumer electronics and electrical vehicles and have several advantages over NiCd and Li-ion batteries. Since the main purpose of the battery is the storage capacity, the maximization of the battery energy density represents significant practical interest. A detailed study of the practical aspects of the application of these new materials in a future generation of NiMH batteries is, therefore, essential. The first NiMH batteries was invented in 1976 in Philips Research laboratory, but became commercially available only in the beginning of 90's (see e.g. Ch. 2 of [9]). The NiMH batteries are alkaline electrical energy storage devices due to the use of a potassium hydroxide (KOH) solution as the electrolyte. Electrically, NiMH batteries are very similar to nickel-cadmium batteries. Rechargeable alkaline storage batteries are very attractive due to several important reasons:

- High electrolyte conductivity allows for high power applications;
- The battery system can be sealed, minimizing maintenance and leakage issues;
- Operation is possible over a wide temperature range;
- Long life characteristics offset higher initial costs compared to other technologies;
- Higher energy density and lower cost per watt or watt-hour (depending on design);
- Non-toxic composition elements.

Commercially available NiMH batteries use conventional $LaNi_5$–based alloys as the MH electrode materials. These batteries have a low storage capacity, around 1100 mAh for AA-size battery. The reason is high density of $LaNi_5$–based alloys (around $8.6 \cdot 10^6$ g/m^3). Recently introduced NiMH batteries have a higher capacity (up to 2600-2700 mAh for AA-zise battery) and this is mostly because of improvements in the battery manufacturing processes (for example, decreasing of "dead" volume of the battery tube), not because of changes in the composition of the MH electrode.

The main goal of the present paper is to provide a theoretical estimation of the energy density of NiMH batteries where newly developed hydrogen storage alloys are used as MH electrode materials. Replacement of the old MH electrode material by the

new prospective alloys together with improving technology of battery manufacturing is a big step in producing of the new generation of the NiMH batteries.

2. Model Description

The processes taking place in the NiMH battery are shown in Fig. 3. The battery consists of two electrodes, *i.e.* a nickel and a hydride electrode. Both electrodes are immersed in strong alkaline solution and electrically insulated by a separator impregnated with a KOH solution [2-4].

During charging divalent Ni is oxidized to trivalent state:

$$Ni(OH)_2 + OH^- \underset{\text{discharging}}{\overset{\text{charging}}{\rightleftharpoons}} NiOOH + H_2O + e^- . \qquad (1)$$

At the same time water is reduced to hydrogen atoms which are absorbed by the hydride-forming electrode material:

$$M + xH_2O + xe^- \underset{\text{discharging}}{\overset{\text{charging}}{\rightleftharpoons}} MH_x + xOH^- . \qquad (2)$$

Hydroxyl ions in the electrolyte are transported from one electrode to another. The reverse reactions take place during discharging.

During overcharging OH^- ions are oxidized and oxygen evolution starts at the Ni electrode. As a result, the partial oxygen pressure inside of the battery starts to rise. Fortunately, oxygen can be transported to the MH electrode where it can be reduced to hydroxyl ions. The overall oxygen reaction can be represented as:

$$4OH^- \underset{\text{MH}}{\overset{\text{Ni}}{\rightleftharpoons}} 2H_2O + O_2 + 4e^- . \qquad (3)$$

The overdischarging reaction takes place when battery is empty. Under this reaction water is reduced at the Ni electrode which also results in a hydrogen pressure built-up inside of the battery. Fortunately, hydrogen can be converted at the MH electrode:

$$2e^- + 2H_2O \underset{\text{MH}}{\overset{\text{Ni}}{\rightleftharpoons}} 2OH^- + H_2 . \qquad (4)$$

To prevent sharp battery voltage dropping and increasing of the internal gas pressure during overcharging and overdischarging the Ni electrode is made capacity-determined electrode. The size of Ni electrode is, therefore, smaller than size of MH one. To avoid increase of hydrogen pressure during overdischarging (Eq. 3) some part of the MH electrode is being charged *a priori*. This amount of hydrogen is called precharge and denoted as Q_{MH}^0 [mAh], see Fig. 3. Denote the normalized hydrogen concentration in the MH electrode at the begin of charging as x^0 and maximal capacity of the MH electrode as $Q_{MH}^{\max}$ [mAh], then

$$x^0 = Q_{MH}^0 / Q_{MH}^{\max} . \qquad (5)$$

Consider the end of charging process. To encourage oxygen recombination and avoid increase of oxygen pressure during overcharging (Eq. 3) some part of the MH electrode remains uncharged (Fig. 3). Denote the normalized hydrogen concentration in the MH electrode at the end of the charging process, when the Ni electrode is fully charged, as $x^{\max}$, then

$$x^{\max} = (Q_{MH}^0 + Q_{Ni}^{\max}) / Q_{MH}^{\max} . \qquad (6)$$

Therefore under normal operation conditions the state of charge of MH electrode varies between x^0 and $1 - x^{\max}$.

State of charge of the battery is the ratio (often expressed in %) between the currently stored amount of electricity (Q_{bat}) and the battery capacity:

$$SoC_{bat} = \frac{Q_{bat}}{Q_{bat}^{\max}}, \tag{7}$$

where $Q_{bat}^{\max} = Q_{Ni}^{\max}$ [mAh] is the battery capacity, the maximal charge which can be reversibly extracted from the battery. Note that from Eqs. 5 and 6 it follows that

$$Q_{Ni}^{\max} = Q_{MH}^{\max}(x^{\max} - x^{0}). \tag{8}$$

Suppose that the battery has been (dis-)charged using reasonably low current. If charge of the battery is changed by the small amount of dq then change in the battery energy (U_{bat}) can be expressed as:

$$dU_{bat} = E_{bat}(q)dq, \tag{9}$$

where E_{bat} is battery voltage. Integration of the elemental energies (Eq. 9) during the battery operation cycle gives the total energy of the battery:

$$U_{bat} = \int_{0}^{Q_{Ni}^{\max}} E_{bat}(q)dq. \tag{10}$$

Obviously, the total NiMH battery voltage is the difference between the voltage of the Ni electrode and that of the MH electrode:

$$U_{bat} = \int_{0}^{Q_{Ni}^{\max}} E_{Ni}(q)dq - \int_{0}^{Q_{Ni}^{\max}} E_{MH}(q)dq, \tag{11}$$

which can be expressed in terms of average voltages:

$$U_{bat} = Q_{Ni}^{\max}(\bar{E}_{Ni} - \bar{E}_{MH}) = Q_{Ni}^{\max}\bar{E}_{bat}, \tag{12}$$

where average voltages of the Ni and MH electrodes respectively are defined as:

$$\bar{E}_{Ni} = \int_0^1 E_{Ni}(x_{Ni})dx_{Ni}; \quad \bar{E}_{MH} = \int_{x^0}^{x^{\max}} \frac{E_{MH}(x_{MH})}{x^{\max} - x^0} dx_{MH}. \tag{13}$$

One of the most important characteristic of the battery is its energy density. Usually two kinds of energy density can be distinguished: volumetric energy density (energy density per battery volume, denoted as d) and gravimetric energy density (energy density per battery mass, denoted as D). These characteristics are defined as

$$d = U_{bat}/V_{bat}; \qquad D = U_{bat}/m_{bat}, \tag{14}$$

where V_{bat} is the total battery volume and m_{bat} is the total battery mass.

To compare two different kinds of NiMH batteries one can compare volumetric and gravimetric energy densities given by Eq. 14 at constant battery volume (with fixed form factor) or at constant battery mass (with fixed weight).

Consider the energy densities at constant battery volume. The total volume of usual NiMH battery is obtained by summation of volumes of all parts of the battery, thus

$$V_{bat} = V_{Ni} + V_{MH} + V_{el} + V_g + V_c, \tag{15}$$

where V_{Ni} is the volume of the Ni electrode; V_{MH} is the volume of the MH electrode; V_{el} is the volume of the electrolyte; V_g is the volume of the gas phase; V_c is the volume of the battery cover (frame) and other “dead” parts.

Suppose that volumes of the electrolyte, gas and battery cover are kept constant. If the total battery volume is also constant then one can write:

$$V_{Ni} + V_{MH} = const\,. \tag{16}$$

Denoting $V_{tot} = V_{Ni} + V_{MH}$ and taking into account Eqs. 8 and 16 one can express volumes of the Ni and MH electrodes:

$$V_{Ni} = \frac{V_{tot} c_{MH} (x^{\max} - x^0)}{c_{Ni} + c_{MH} (x^{\max} - x^0)}; \qquad V_{MH} = \frac{V_{tot} c_{Ni}}{c_{Ni} + c_{MH} (x^{\max} - x^0)}, \tag{17}$$

where $c_i = Q_i^{\max} / V_i$ [mAh/m^3], $i = Ni, MH$, is the capacity of the i-th electrode per unit of volume. Expressing capacity of the Ni electrode, substituting it into energy density Eq. 14 and taking into account definition Eq. 12 one can obtain energy densities of the battery at constant volume:

$$d_V = \overline{E}_{bat} \frac{V_{tot}}{V_{bat}} \frac{c_{Ni} c_{MH} (x^{\max} - x^0)}{c_{Ni} + c_{MH} (x^{\max} - x^0)}; \qquad D_V = \overline{E}_{bat} \frac{V_{tot}}{m_{bat}} \frac{c_{Ni} c_{MH} (x^{\max} - x^0)}{c_{Ni} + c_{MH} (x^{\max} - x^0)}. \tag{18}$$

Now consider the energy densities at constant battery mass. Similarly to the Eq. 15 the total battery mass can be expressed as follows:

$$m_{bat} = m_{Ni} + m_{MH} + m_{el} + m_c\,. \tag{19}$$

Suppose that the masses of the electrolyte and battery cover are kept constant. If the total mass of the battery is also constant then one can write:

$$m_{Ni} + m_{MH} = const\,. \tag{20}$$

Denoting $m_{tot} = m_{Ni} + m_{MH}$ and taking into account Eqs. 8 and 20 one can express masses of the Ni and MH electrodes:

$$m_{Ni} = \frac{m_{tot} C_{MH} (x^{\max} - x^0)}{C_{Ni} + C_{MH} (x^{\max} - x^0)}; \qquad m_{MH} = \frac{m_{tot} C_{Ni}}{C_{Ni} + C_{MH} (x^{\max} - x^0)}, \tag{21}$$

where $C_i = Q_i^{\max} / m_i$ [mAh/kg], $i = Ni, MH$, is the capacity of the i-th electrode per unit of mass. Expressing capacity of the Ni electrode, substituting it into energy density Eq. 14 and taking into account definition Eq. 12 one can obtain energy densities of the battery at constant mass:

$$d_m = \bar{E}_{bat} \frac{m_{tot}}{V_{bat}} \frac{C_{Ni} C_{MH} (x^{\max} - x^0)}{C_{Ni} + C_{MH} (x^{\max} - x^0)}; \qquad D_m = \bar{E}_{bat} \frac{m_{tot}}{m_{bat}} \frac{C_{Ni} C_{MH} (x^{\max} - x^0)}{C_{Ni} + C_{MH} (x^{\max} - x^0)}. \tag{22}$$

3. Results And Discussion

To estimate energy characteristics of the battery with new lightweight hydride-forming materials as MH electrode the standard setup of Philips rechargeable R6NM battery with capacity 2600 mAh has been selected. The volumetric energy density of this battery is about 410 Wh/l and corresponding gravimetric energy density is about 106 Wh/kg.

The open-circuit voltage (OCV) of the Ni electrode is important part of the model developed in section 2 (see e.g. Eq. 12). In the reasarch group of P. Notten a number of measurements was made to find OCV of Ni electrode as function of the corresponding state of charge. Specifically, the OCV of commercial 1100 mAh AA-size NiMH battery (HHR110AAOK, Matsushita Battery Industries, Japan) was measured by two different methods: by extrapolation of different voltage-current curves to zero current and by the voltage relaxation method, when at given depth-of-charge the OCV is determined as voltage at the end of the relaxation period (see [10,11] for details). Using total equilibrium battery voltage and equilibrium voltage of the MH electrode the OCV of the Ni electrode can be restored:

$$E_{Ni} = E_{bat} - E_{MH}. \tag{23}$$

The average voltage of the Ni electrode then was calculated by Eq. 13. Since composition of the Ni electrode is the same in all NiMH batteries, that average voltage can be used without restrictions for other NiMH batteries.

It was assumed that the MH electrode in the Philips battery is made of classical LaNi-based hydride forming material, similar to those of the old battery [10,11]. Advance in capacity of the Philips battery is achieved because of implementation of new industrial technologies. In the Philips battery cover, separator and other parts are thinner than in the old battery and, therefore, there is more space for electrodes. Thus it was assumed that ratios $V_{tot}/V_{bat} = const$ and $m_{Ni}/m_{MH} = const$ remain the same for both batteries. Precharge of the MH electrode of normal NiMH battery (see Eq. 5) was estimated to be around 16% of electrode capacity, while maximul achievable state of charge (see Eq. 6) constitutes about 73% of electrode capacity. Measured and calculated characteristics of the Philips battery are represented in the Table 1.

The new prospective lightweight $Mg_{0.80}Sc_{0.20}$ hydride-forming alloy recently invented in the Philips Research Laboratory has extremely large capacity 1740 mAh/g (see [7,8]). Various properties of that alloy were measured. The OCV voltage was measured electrochemically in a three-electrode setup using Maccor M2300 battery tester. Electrochemical impedance spectroscopy (EIS) has been done on Autolab PGSTAT30. The density of the $Mg_{0.80}Sc_{0.20}$ alloy was estimated to be about $2 \cdot 10^6\ g/m^3$. Suppose now that this material was used as an MH electrode material for *advanced* NiMH battery. Model derived in section 2 can explain properties of such advance battery, in particular to find volumetric and gravimetric energy densities. Table 2 gives a summary of various characteristics of the advanced NiMH battery in assumptions of "constant volume" battery and "constant mass" battery. Comparison with standard R6NM Philips battery is also provided. The results represented in the Table 2 have been obtain using Eqs.13, 17, 18, 21 and 22 of the section 2. It was assumed that the volume of the electrolyte in the advanced battery is proportional to the volume of electrodes. This assumption reflects the fact that one needs more electrolyte to make wet larger electrode surface. Fig. 4 illustrates OCV of MH electrode (a) and capacity-determining Ni electrode (b).

To facilitate comparison between standard and advanced batteries the gain functions were introduced, namely:

$$g_i = \frac{d_i^{adv}}{d_i^{ref}} - 1; \quad G_i = \frac{D_i^{adv}}{D_i^{ref}} - 1, \tag{24}$$

where upper-indices “ref” and “adv” refer to reference (standard Philips R6NM battery) and advanced (Philips-like battery with the new $Mg_{0.80}Sc_{0.20}$ hydride-forming material as the MH electrode) batteries accordingly; lower index i, $i = V, m$ indicates setup with “constant volume” battery and “constant mass” battery accordingly.

Consider “constant volume” battery setup. Results imply that introduction of new materials gives no gain in volumetric energy density. However gain in gravimetric energy density is G_V is 59%. Apparently, implementation of the new $Mg_{0.80}Sc_{0.20}$ material as MH electrode makes battery lighter and therefore results in gravimetric energy density gain.

Simulation results for “constant volume” battery suggest that main advantage of the new $Mg_{0.80}Sc_{0.20}$ material is its light weight. Therefore it is expected that case of “constant mass” battery will give even higher gain in gravimetric energy density. These expectations are confirmed by the results represented in Table 2. The gravimetric gain function reaches impressive 80% value. Corresponding energy density is equal to 190 Wh/kg. At the same time some volumetric gain is observed (around 5%) and one may wonder why does it happened? The explanation can be found in rows 1-3 of Table 2 where expected volumes of electrodes are reported. The expected volume of Ni electrode V_{Ni} constitutes larger fraction of total battery volume V_{tot} in case of “constant mass”, in comparison with “constant volume”. Therefore the “inactive” volumes (gas volume, electrolyte volume ect.) are smaller and therefore the volumetric gain is higher than for the case of “constant volume”.

It is instructive to find a limits of energy densities when technology is assumed perfect and volumes of electrolyte and “dead” parts of the battery described by the Eq. 15 are negligible, thus $V_{tot} = V_{bat}$. Then “technologically limiting” value of volumetric energy density can be derived from first of Eq. 18 as

$$d^{\max} = \bar{E}_{bat} \frac{c_{Ni} c_{MH} (x^{\max} - x^0)}{c_{Ni} + c_{MH} (x^{\max} - x^0)}. \quad (25)$$

Similarly the “technologically limiting” value of gravimetric energy density is obtained from second of Eqs.18 assuming $m_{tot} = m_{bat}$, thus

$$D^{\max} = \bar{E}_{bat} \frac{C_{Ni} C_{MH} (x^{\max} - x^0)}{C_{Ni} + C_{MH} (x^{\max} - x^0)}. \quad (26)$$

“Technologically limiting” values of energy densities for constant volume and constant mass are represented in rows 13 and 18 of the Tables 2. Interesting to point out, that especially gravimetric energy density of the new battery (190 Wh/kg) is rather close to the “technologically limiting” value (228 Wh/kg). That indicates significant progress in the battery technology but also suggests that further significant gain in energy density can be made only using the new electrode materials, such as MgSc-based alloys.

From the simulation results one can conclude that application of the new $Mg_{0.80}Sc_{0.20}$ lightweight hydride forming material will produce AA-size battery with expected capacity 3045 mAh. The estimated value of gravimetric energy density ~190 Wh/kg is somewhat higher than values reported for majority of currently available lithium batteries (sources [12-13] report values in the range of 100-200 Wh/kg). One may conclude, that application of Mg-Sc-based alloys will overcome the largest disadvantage of existing NiMH batteries: low specific energy.

Although the results of the Mg-Sc alloy look promising it will never be used on a large scale because of the high costs of metallic Sc. However, it has cheaper alternatives. Recently new binary (*e.g.* Mg-Ti) and ternary (*e.g.* Mg-Ti-Al) alloys have been developed by the group of Prof. Dr. P.H.L. Notten in the 'Portable Energy' laboratory of Philips NATLab and demonstrated almost the same capacity as Mg-Sc (see [14]). These new alloys are low cost and, therefore, suitable for large scale implementation. Replacement of the old MH electrode material by the new ones together with

improvements in the manufacturing technology constitutes a big step towards a new generation of NiMH batteries.

As we already pointed out, the application of new lightweight hydrogen storage materials gives the maximal effect if it is used on a large scale. In contrast to old NiCd and modern Li-ion batteries the new materials are non-toxic and not sensitive to the strong outdoor conditions. One of the attractive applications of the new NiMH batteries is large battery packs, which can be charged by primary energy sources such as solar, tides, wind, etc. For example, large NiMH packs using part of the energy generated by solar elements during the daylight and work as an autonomous energy source at night. Also, the new NiMH batteries can be efficiently included to Combined Heat and Power (CHP) technology as additional energy storage.

4. Conclusions

The new mathematical model to estimate volumetric and gravimetric energy densities (specific energies) of the rechargeable NiMH batteries has been proposed. Using this model the application of the new prospective $Mg_{0.80}Sc_{0.20}$ hydride forming material as a MH electrode in standard setup of Philips rechargeable R6NM battery has been investigated. The new material is characterized by high hydrogen storage capacity (1740 mAh/g) and light weight (its density is $2 \cdot 10^6$ g/m^3).

From simulation results it follows that application of new $Mg_{0.80}Sc_{0.20}$ alloy gives 59% gain in gravimetric energy density if it is used in normal AA-size battery (“constant volume” battery) and provides expected capacity of 3045 mAh. The energy density of the battery which has the same weight (“constant mass” battery) as normal AA-size battery but does not have volume limitations also was estimated. In this case higher gains were achiebed, *i.e.* 5% in volumetric energy density and 88% in gravimetric one. It is interesting to note that the gravimetric energy density in this case is higher than those for the majority of currently available lithium-ion batteries. Although the results of the Mg-Sc alloy look promising it will never be used on a large scale because of the high costs of metallic Sc. However, new binary (*e.g.* Mg-Ti) and ternary (*e.g.* Mg-Ti-Al) alloys have been developed by the group of Prof. Dr. P.H.L. Notten in the 'Portable Energy'

laboratory of Philips NATLab and demonstrated almost the same capacity as Mg-Sc. As these new alloys are low cost they are suitable for a large scale implementation.

References

1. Y. Fukai, "*The Metal-Hydrogen System*", Springer-Verlag, Berlin Heidelberg, 1993.
2. P.H.L. Notten, "*Rechargeable Nickel-MetalHydride batteries: a successful new concept*", Chapter 7 in *"Interstitial intermetallic alloys"*, NATO ASI Series E 281 (1995) 151, Edts. F. Grandjean, G.J. Long and K.H.J. Buschow, ISBN 0-7923-3299-7.
3. P.H.L. Notten, "*Rechargeable Batteries: Efficient Energy Storage Devices for Wireless Electronics*", Chapter 5.3 in "*Hardware Technology Drivers of Ambient Intellegence*", Dordrecht, Springer (2006), Ed. S. Mukherjee, ISBN 978-1-4020-4197-6.
4. P.H.L. Notten and M. Latroche, "*Nickel MetalHydride batteries: a successful application of hydrogen storage materials*", Chapter 5.4 in "*Hydrogen the energy carrier of the future*", Wiley, London, in press (2005).
5. L. Schlapbach and A. Zuttel, Hydrogen storage materials for mobile applications, Nature, 414, 353, 2002.
6. J.D. Power and Associates-LMC Automotive Forecasting Services, "*The Hybrid-Electric Vehicle Outlook*" 02/03/05.
7. R.A.H. Niessen, "*Electrochemical hydrogen storage in lightweight electrode materials*", PhD thesis, 2006.
8. P. Kalisvaart, P. Vermeulen, A. Ledovskikh, D. Danilov and P.H.L. Notten, The electrochemistry and modeling of hydrogen storage materials, *Journal of Alloys and Compounds*, 2006, in press, available online 11 December 2006.
9. V. Pop, H.J. Bergveld, D. Danilov, P.P.L. Regtien, P.H.L. Notten, "*Battery Management Systems: Accurate State-of-Charge Indication for Battery-Powered Applications"*, Springer, in print.
10. I. Snihir, W. Rey, E. Verbitskiy, A. Belfadhel-Ayeb, P.H.L. Notten, Journal of Power Sources, 159 (2), 1484, 2006.
11. A. Ayeb, W. M. Otten, A. J. G. Mank, P.H.L. Notten, to be published in the Journal of the Electrochemical Society, 153 (11), A2055, 2006.

12. M. Broussely, “Lithium-Ion batteries for EV, HEV and other applications”, Chapter 21 in Lithium Batteries, Science and Technology, G.Nazri and G. Pistoia, eds., Kluwer publishers, Boston, 2004, ISBN 1-4020-7628-2.
13. D. MacArthur, “Current issues and market trends of Li-ion batteries for consumer applications”, Chapter 23 in Lithium Batteries, Science and Technology, G.Nazri and G. Pistoia, eds., Kluwer publishers, Boston, 2004, ISBN 1-4020-7628-2.
14. P. Vermeulen, E.F.M.J. van Thiel, P.H.L. Notten, Ternary MgTiX-alloys: A promising route towards low temperature, high capacity, hydrogen storage materials, Chemistry of Materials, submitted (2007).

FIGURE CAPTIONS

Fig. 1. The dynamic of projected sales growth of HEV in the US.

Fig. 2. Capacity of LaNi-based and new MgSc compounds.

Fig. 3. General scheme of rechargeable NiMH battery.

Fig. 4. OCV-s of MH (a) and Ni (b) electrodes.

Table. 1. Design and calculated parameters of the R6NM Philips NiMH battery.

Description	Notation	Value	Dimension
Ni electrode:			
- Density	ρ_{Ni}	$3.65 \cdot 10^6$	**g/m^3**
- Voltage	$\overline{E}_{Ni}$	0.298	**V**
- Weight	m_{Ni}	9.195	**g**
- Capacity	$Q_{Ni}^{\max}$	2600	**mAh**
MH electrode			
- Density	ρ_{MH}	$8.00 \cdot 10^6$	**g/m^3**
- Precharge	Q_{MH}^0	730	**mAh**
- Weight	m_{MH}	15.719	**g**
Complete battery:			
- Battery volume	V_{bat}	7.697	**ml**
- Electrolyte volume	V_{el}	2.390	**ml**
- Weight	m_{bat}	29.850	**g**
- Total electrode volume	$\boldsymbol{V_{tot}}$	**4.484**	**ml**

Table. 2. Simulated values of various characteristics of the new NiMH battery using $Mg_{0.80}Sc_{0.20}$ prospective hydride-forming alloy as the MH electrode.

N	Battery characteristics	Philips R6NM	Constant volume	Constant mass
1	V_{Ni}, *ml*	*2.519*	2.944	5.312
2	V_{MH}, *ml*	*1.965*	1.540	2.779
3	V_{bat}, *ml*	*7.697*	7.697	13.23
4	m_{Ni}, *g*	*9.195*	10.74	19.39
5	m_{MH} ,*g*	*15.72*	3.061	5.524
6	m_{bat}, *g*	*29.85*	18.74	29.85
7	$\overline{E}_{MH}$, *V*	*-0.92*	-0.736	-0.736
8	E_{bat} , *V*	*1.212*	1.034	1.034
9	d_V, *Wh/l*	*410*	410	---
10	g_V, *%*	*0*	0	---
11	D_V, *Wh/kg*	*106*	168	---
12	G_V, *%*	*0*	58.71	---
13	d^{max}, *Wh/l*	*704*	704	---
14	d_m, *Wh/l*	*410*	---	430
15	g_m, *%*	*0*	---	4.64
16	D_m, *Wh/kg*	*106*	---	190
17	G_m, *%*	*0*	---	80
18	D^{max}, *Wh/kg*	*127*	---	228
19	C_{bat}, *mAh*	*2600*	3045	5490

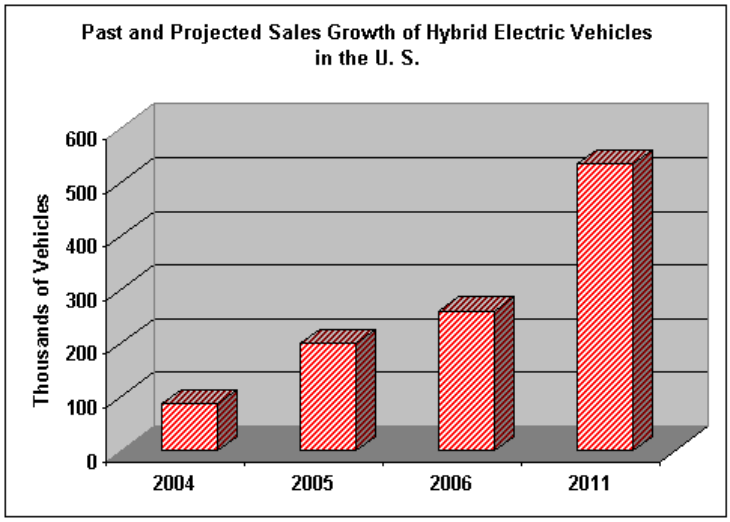

Fig. 1. The dynamic of projected sales growth of HEV in the US.

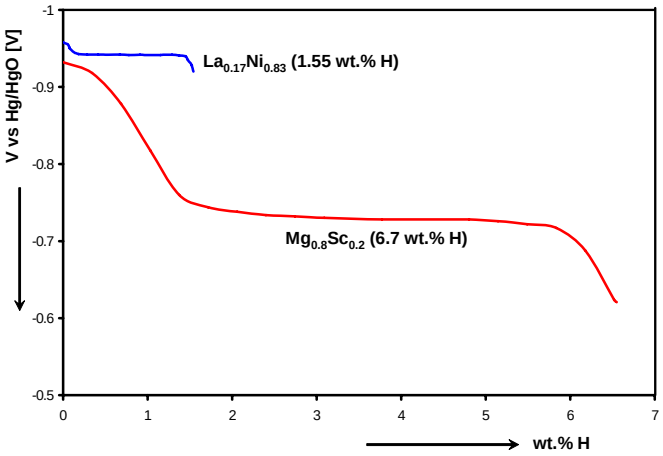

Fig. 2. Capacity of LaNi-based and new MgSc compounds.

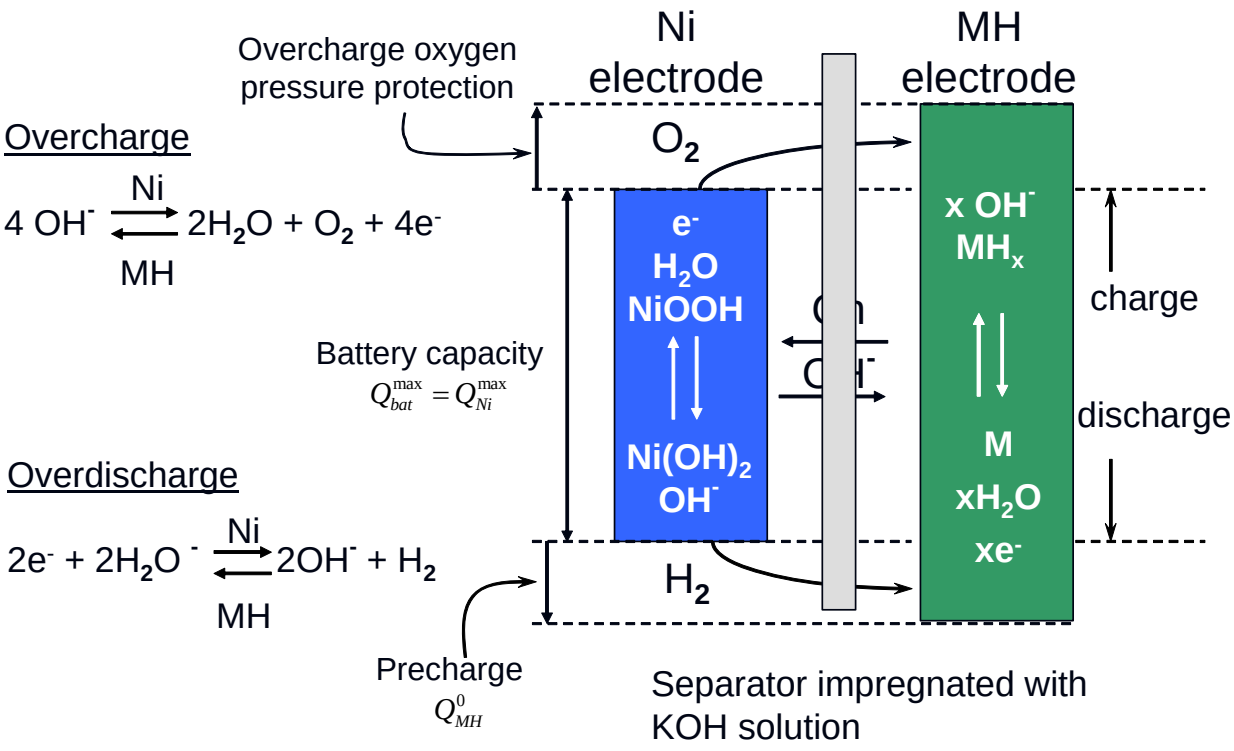

Fig. 3. General scheme of rechargeable NiMH battery.

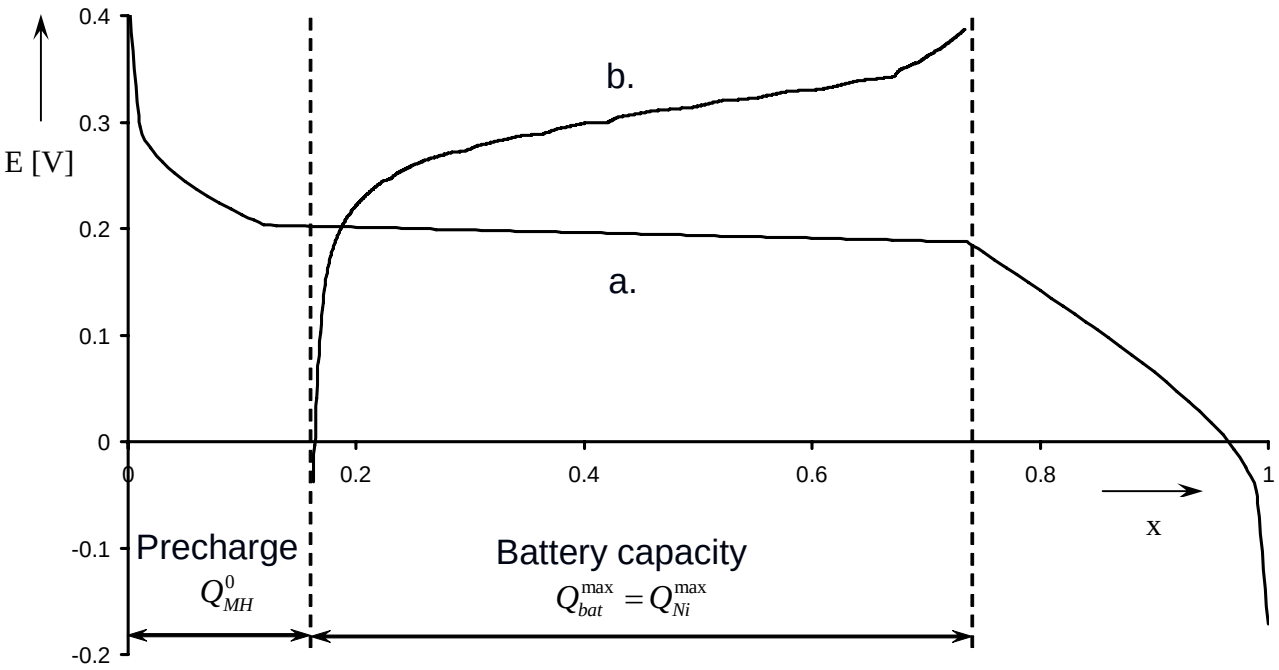

Fig. 4. OCV-s of MH (a) and Ni (b) electrodes.