AMTC Letters
Vol. 1 (2008)



# Modeling of the Structure of Nickel Hydroxide

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Nickel hydroxide is an important material with significant electrochemical applications, such as for the positive electrodes in Ni-H batteries. The active compounds within these electrodes are $Ni(OH)_2$ and NiOOH phases. However, it is reported that the electrochemical cycling between these phases involves the formation of other phases as well[1-2]. The relationship between some of these hydroxides and oxyhydroxide phases is given in Figure 1 as a Bode diagram[3,4]. As shown in the diagram, $\alpha$-$Ni(OH)_2$, $\beta$-$Ni(OH)_2$, $\beta$-NiOOH, and $\gamma$-NiOOH phases are all part of the electrochemical cycle. $\beta$-$Ni(OH)_2$, which adopts a $CdI_2$-type structure, is reportedly the most stable crystalline form of nickel hydroxide. The $\alpha$-phase, may contain significiant amounts of absorbed anions or water, and the structure has been observed to show very broad XRD peaks indicative of disorder. It is reported[5] that $\alpha$-nickel hydroxide is a general label for a large set of disordered $Ni(OH)_2$ structures and does not represent a well defined polymorph of $Ni(OH)_2$. The structure is unstable in alkaline media. Experimental investigations performed in our group have shown that the structure of $Ni(OH)_2$ changes from $\alpha$- to $\beta$- on aging in the synthesis solution. The structure of $\alpha$ phase can be reformulated as $Ni(OH)_{2-x}\ A^{n-}_{x/n}\ mH_2O$ ($A^{n-}$ is the anion) where $x$ can vary between 0.05 and 0.4 and $m$=0.6-1 depending upon the method of preparation and the work up [5]. These phases are non-stoichiometric, hydroxyl deficient, and include a variety of anions in the interlayer region along with water molecules (Figure 2).

Recently it has been reported[5] that a new phase of nickel hydroxide exists, identified as interstratified or an IS phase, produced by the interstratifications of alpha and beta phases. The existence of all these phases with distinct crystallographic sizes and oxidation states makes the chemistry and crystal structure of nickel hydroxide very complicated, but potentially useful in several advanced applications.

In order to better understand the crystalline structure formation and its further evolution we have initiated the present computer simulation study. Initially, we have simulated the structure of $\beta$- $Ni(OH)_2$ using force field parameters optimized against first principle (DFT) calculations, which are in good agreement with experimental values. We have also simulated structural changes of nickel hydroxide using molecular dynamics (MD). The study is continuing and we look forward to reporting detailed results in this presentation. We expect that the theoretical studies will provide a solid understanding of the complicated crystal chemistry of nickel hydroxide, including the interlamellar hydration.

References

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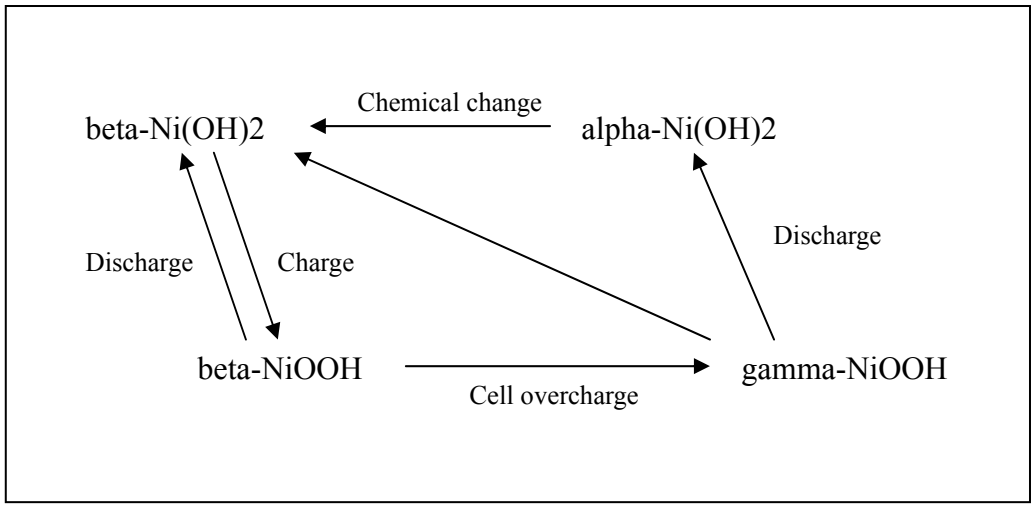


FIG. 1. Bode Diagram

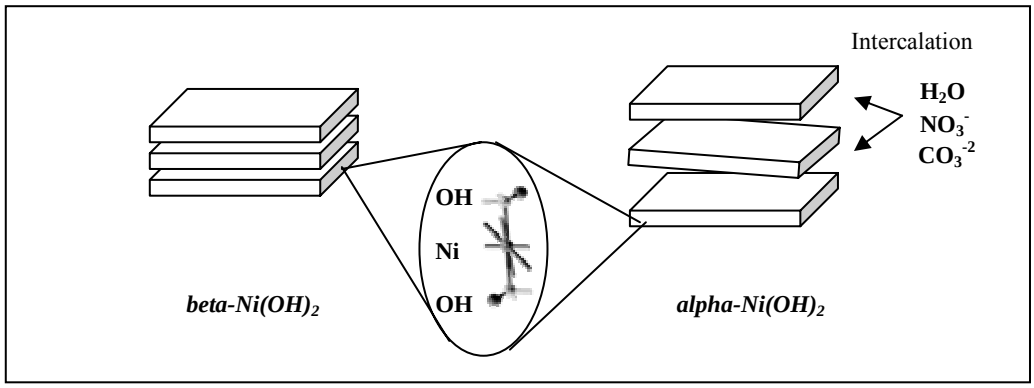


FIG. 2. Models of alpha- and beta- Nickel Hydroxide