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Erratum

Erratum to "The possibility of voltage prediction from the Coulomb potential created by the atoms of a cathode active material for Li ion cells" [J. Power Sources 90 (2000) 116–125]☆

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The publisher and authors regret errors which appeared in the above-mentioned article.

The plateau voltage shown in Figs. 1, 5, and 6 were wrong. The authors have to compare the Gibbs free energy to evaluate two-phase region.

They obtained the following equation.

$$E = E^{\circ} + Ky - \left(\frac{RT}{F}\right)\ln\left(\frac{y}{1-y}\right) \qquad (14)$$

where,

$E^{\circ} = 3.879$ V, $K = 1.011$ V and $y = x/0.25$ for $0 < x < 0.25$,

$E^{\circ} = 3.179$ V, $K = 1.095$ V and $y = (x - 0.25)/0.25$ for $0.25 < x < 0.50$,

$E^{\circ} = 3.346$ V, $K = 1.095$ V and $y = (x - 0.5)/0.25$ for $0.50 < x < 0.75$,

$E^{\circ} = 2.648$ V, $K = 1.011$ V and $y = (x - 0.75)/0.25$ for $0.75 < x < 1$.

Because K should have the same value, they used 1.011 V for all the K. From Eq. (14), Eqs. (2) and (3), the corresponding Gibbs free energy is

$$G = -\frac{F}{4} \times \left\{E_i^{\circ} y + \frac{K_i}{2}y^2 - \frac{RT}{F}[y\ln y + (1-y)\ln(1-y)] + C_i\right\}$$

where,

$E_1^{\circ} = 3.879$ V, $K_1 = 1.011$ V, $C_1 = 0$ and $y = x/0.25$ for $0 < x < 0.25$,

$E_2^{\circ} = 3.179$ V, $K_2 = 1.011$ V, $C_2 = -(E_1^{\circ} + K_1/2)$ and $y = (x - 0.25)/0.25$ for $0.25 < x < 0.50$,

$E_3^{\circ} = 3.346$ V, $K_3 = 1.011$ V, $C_3 = C_2 - (E_2^{\circ} + K_2/2)$ and $y = (x - 0.5)/0.25$ for $0.50 < x < 0.75$,

$E_4^{\circ} = 2.648$ V, $K_4 = 1.011$ V, $C_4 = C_3 - (E_3^{\circ} + K_3/2)$ and $y = (x - 0.75)/0.25$ for $0.75 < x < 1$.

If Li^+ ordering does not occur, G is

$$G = -F\left\{3.879x \frac{-0.220x^2}{2} - \frac{RT}{F}[x\ln(x) + (1-x)\ln(1-x)]\right\}$$

The relation is shown in Fig. E-1. There are three tangential lines, which show phase separation at $0 < x < 0.25$, $0.25 < x < 0.75$, and $0.75 < x < 1$. From Eq. (2), the potential of the phase separation area is −(slope of the tangential line). Therefore, the bold curve shown in Fig. 4 was wrong. The correct figure is shown as Fig. E-2. There were the same mistakes in Figs. 5 and 6 as in Fig. 4. The bold curve in Fig. 6 should be 3.040 V ($0 < x < 0.25$), 2.478 V ($0.25 < x < 0.75$) and 1.847 V ($0.75 < x < 1$). In order to appear single phase, the G at $x = 0.5$ and $x = 0.75$ have to be larger than the corresponding G of no ordering stage. The authors are now investigating the improved calculation to obtain a better result.

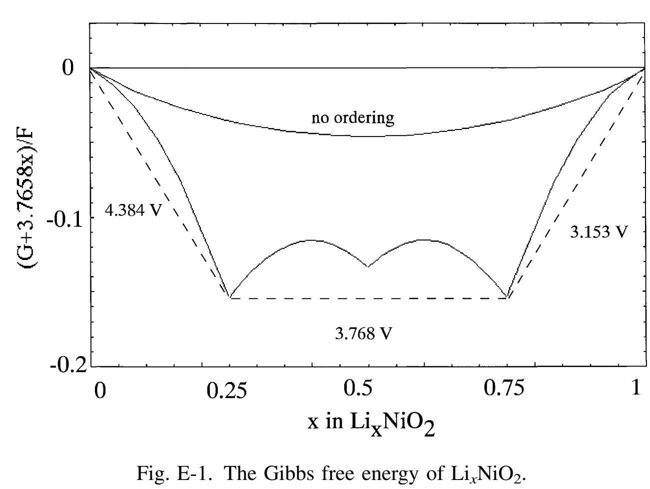

Fig. E-1. The Gibbs free energy of Li_xNiO_2.

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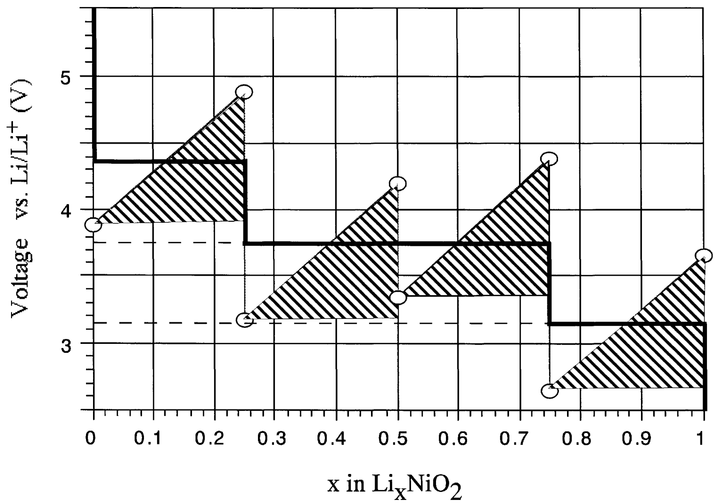

Fig. E-2. The calculated voltage of Li_xNiO_2.