

Electrochemical Behavior of Al(III) and Formation of Different Phases Al-Ni Alloys deposits from LiCl-KCl-AlCl₃ Molten Salt

Yaru Peng, Zeng Chen *, Ying Bai, Qingqing Pei, Wei Li, Chunli Diao, Xijin Li, Shengjun

Li * and Shaokang Dong

Table S1. Standard Gibbs free energies of formation for Al-Ni intermetallic compounds.

Reaction	Equation for ΔG_f^0	$-\Delta G_f^0 / \text{kJ}\cdot\text{mol}^{-1}$
$\text{Al(III)} + 1/3 \text{ Al}_3\text{Ni}_2 + 3 \text{ e} = 2/3 \text{ Al}_3\text{Ni}$	$\frac{3}{2} (-3 F \Delta E_6 + \frac{1}{3} \Delta G_{f, \text{Al}_3\text{Ni}_2}^0)$	318.34
$\text{Al(III)} + 2 \text{ AlNi} + 3 \text{ e} = \text{Al}_3\text{Ni}_2$	$-3 F \Delta E_5 + 2 \Delta G_{f, \text{AlNi}}^0$	437.08
$\text{Al(III)} + 1/2 \text{ Ni}_5\text{Al}_3 + 3 \text{ e} = 5/2 \text{ AlNi}$	$\frac{2}{5} (-3 F \Delta E_4 + \frac{1}{2} \Delta G_{f, \text{Ni}_5\text{Al}_3}^0)$	162.09
$\text{Al(III)} + 5/4 \text{ AlNi}_3 + 3 \text{ e} = 3/4 \text{ Ni}_5\text{Al}_3$	$\frac{4}{3} (-3 F \Delta E_5 + \frac{5}{4} \Delta G_{f, \text{AlNi}_3}^0)$	555.75
$\text{Al(III)} + 3 \text{ Ni} + 3 \text{ e} = \text{AlNi}_3$	$-3 F \Delta E_6$	208.41

Table S2. The partial molar Gibbs free energies and activities of Al in two-phase coexisting states at 753 K.

Plateau	E/V (vs. Pt)	$\Delta E/V$ (vs. $\text{Al(III)}/\text{Al}$)	$-\Delta G_{\text{Al}}/\text{kJ}\cdot\text{mol}^{-1}$	$\alpha_{\text{Al, Ni}}$
I	-1.660 ± 0.003			
II	-1.432 ± 0.003	0.23 (in the co-existing Al_3Ni and Al_3Ni_2 phases)	66.58	2.41×10^{-5}
III	-1.271 ± 0.005	0.39 (in the co-existing Al_3Ni_2 and AlNi phases)	112.89	1.47×10^{-8}
IV	-1.219 ± 0.002	0.44 (in the co-existing AlNi and Ni_5Al_3 phases)	127.36	1.46×10^{-9}
V	-1.117 ± 0.006	0.54 (in the co-existing Ni_5Al_3 and AlNi_3 phases)	156.31	1.43×10^{-11}
VI	-0.938 ± 0.006	0.72 (in the co-existing AlNi_3 and Al phases)	208.41	3.48×10^{-15}