

Low temperature synthesis and catalytic activity of Ni-Al solid solution and Ni₃Al intermetallic:
combined experimental and first-principles study

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The Ni-Al Alloy has received much attention as an anode material for high temperature fuel cells due to its high creep resistance and redox stability. However, its high production cost (Note that the high temperature and extremely low oxygen partial pressure are required for the conventional synthesis of Ni-Al alloy) has retarded the early commercialization of Ni-Al alloys. Thus, the dramatic reduction in the cost of preparing Ni-Al alloy is imperative for the successful application of Ni-Al alloy to the anode materials.

In this talk, we present a cost-effective synthesis process of Ni-Al alloy, which is based on the issued USA/KOREA patents commercialized by fuel cell research center, KIST. In addition, using density functional theory (DFT) calculations, we examine the role of Al on Ni-Al alloys in determining H₂S poisoning/carbon coking resistance.