ECP 2025 Conference

The 4th International Electronic Conference on Processes

20–22 October 2025 | Online

MDPI

The use of lanthanum-based intermetallic compounds as a catalyst in the electrochemical process of ammonia synthesis

Sergey Nesterenko[1], Ilja Chernyshev[1], Irina Kuznetsova[1], Dmitry Kultin[1], Olga Lebedeva[1], Leonid Kustov[1,2]

[1]Department of Chemistry, Lomonosov Moscow State University, Moscow, 119991, Russia;

[2]N.D. Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences, Leninsky Prospect 47, Moscow, 119991, Russia

INTRODUCTION & AIM

Intermetallic compounds (IMCs) have an ordered structure of active sites with a regulated electronic structure and atomic ensemble size. IMCs can be used to create catalysts with high practical performance, including for complex and environmentally friendly electrochemical reactions such as nitrogen reduction (NRR), nitrate conversation (NO_3RR), and nitrite reduction (NO_2RR), which could potentially could replace the industrial Haber-Bosch process. A current priority is the development of efficient electrocatalysts using inexpensive non-precious metals with partial or complete replacement of precious metals [Ref 1]. A promising strategy is the combination of transition metals with p-block elements to tune the adsorption of nitrates/protons and essentially improve the NO_3RR performance. Compared to solid solution alloys, intermetallic compounds (IMCs) possess uniformly dispersed active sites, controllable electronic structure, and excellent stability. To achieve this goal, it is proposed to use IMCs based on non-precious metals or with the addition of some precious metals to maintain high efficiency [Ref 2].

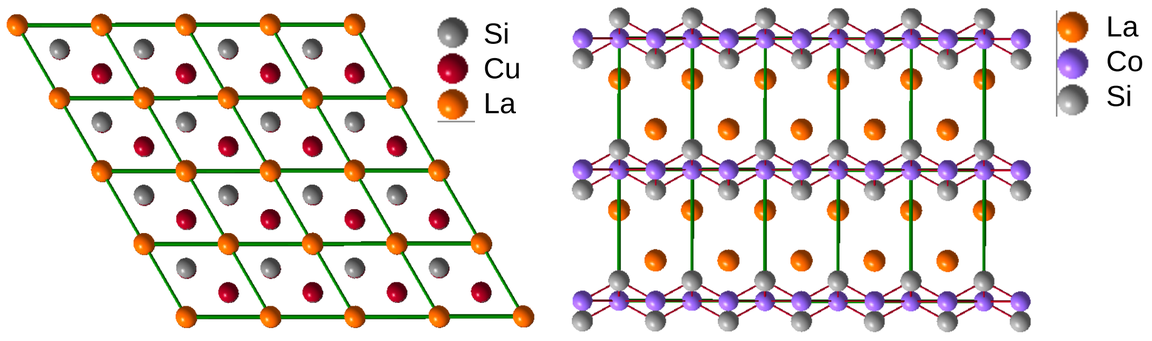
NO_3RR is of particular interest, as it allows for the production of a valuable product and addresses the problem of purifying wastewater from nitrogenous pollutants. Recent research shows that intermetallic compounds open up new possibilities for creating highly efficient catalytic systems for this process. In this work, studies on the use of La-containing IMCs as catalysts in the NO_3RR reaction were conducted for the first time.

MATERIALS & METHODS

La (99.8 %) | Cu (99.999 %) | Co (99.95 %) | Si (99.999 %)

→ LaCuSi, LaCoSi

Crystal structure and Synthesis



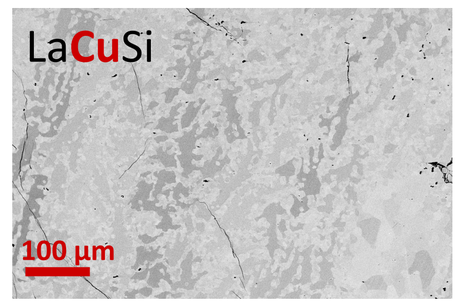
- The arc melting in argon atmosphere (Arc Melting system AM,BUEHLER)
- The heat treatment time at 800 °C (150 hours)

RESULTS & DISCUSSION

Results of X-ray and EDX analyses

LaCuSi → Phases → LaCuSi, La_2CuSi_3

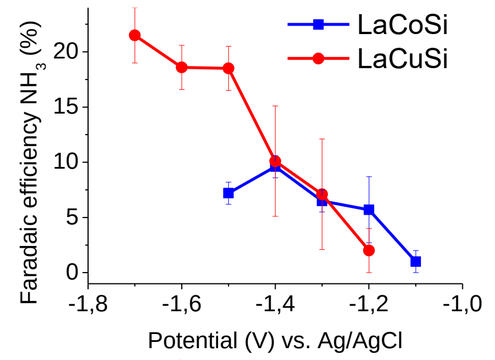
LaCoSi → Phase → LaCoSi



Analysis of Faradaic efficiency

$NO_3^- + 6H_2O + 8e^- = NH_3 + 9OH^-$, $E^0 = 0.88$ В отн. RHE [Ref 3]

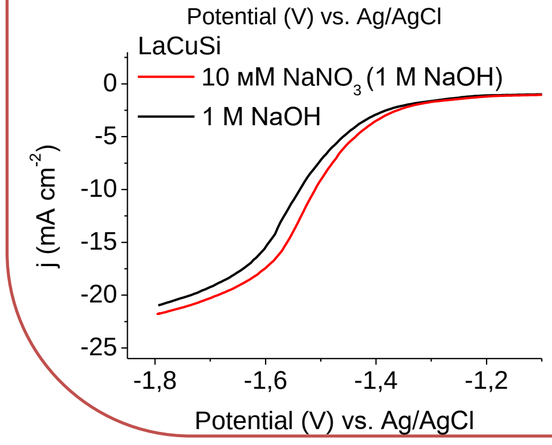
The sample	Potential for reaction NO_3RR (vs. Ag/AgCl)						
	-1.1 V	-1.2 V	-1.3 V	-1.4 V	-1.5 V	-1.6 V	-1.7 V
LaCoSi	1.0	5.7	6.5	9.6	7.2	–	–
LaCuSi	–	2.0	7.1	10.1	18.5	18.6	21.5

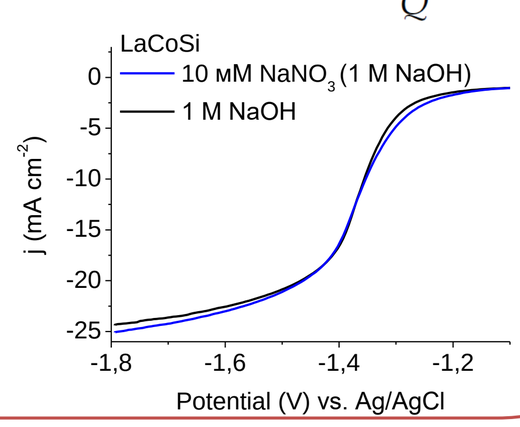


Faradaic efficiency

- $n(NH_3)$ denotes the amount (mol) of NH_3
- F is the Faradaic constant (96,485 C mol^{-1})
- Q is the total charge passed through the electrode
- 8 is the number of electron (n) transfers required to form 1 mol of ammonia

$$FE(NH_3) = \frac{8 \times F \times n(NH_3)}{Q}$$





CONCLUSION

- Ternary intermetallic alloys (IMCs) based on lanthanum and non-precious metals Cu(Co) and Si were synthesized. For the first time, bi- and multicomponent alloys based on lanthanum (containing IMCs) were tested in NO_3RR.
- The use of IMC-based electrocatalysts is promising, as the conducted study demonstrated good values of both Faradaic efficiency (FE) and ammonia yield. LaCuSi compound demonstrate higher efficiency compared to La-based IMCs containing Co.
- It was found that when using the LaCuSi alloy as a cathode, the predominant reaction is nitrate reduction. In the case of LaCoSi alloy as a cathode, the reactions of ammonia production from nitrates and the hydrogen evolution reaction occur simultaneously.

FUTURE WORK / REFERENCES

[1] Liu D., Qiao L., Peng, S., Bai H., Liu C., Ip W.F., Lo K.H., Liu H., Ng K.W., Wang S. et al. *Adv. Funct. Materials* **2023**.

[2] Kuznetsova I., Kultin D., Lebedeva O., Nesterenko S., Murashova E., Kustov L. *Int. J. Mol. Sci.* **2025,** 26,1650**.**

[3] Zhang K., Zhang K.,. Liu Y ., Pan Z., Xia Q., Huo X ., Esan O., Zhang X., An L. *EES Catalysis*. **2024,** 2,727.

Acknowledgments: The research was carried out at the expense of the grant of Russian Science Foundation (RSF) No 25-29-00488, https://rscf.ru/en/project/25-29-00488/