Unlocking the Mystery of Catalytic Design for Methanol Steam Reforming

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Perovskite-type oxide materials (ABO_3) are a very versatile class of materials. Their ability to exsolve metallic nanoparticles on their surfaces has drawn an increasing interest of the scientific community for their application as catalysts in complex reaction conditions. Via doping the A- and B-sites of these materials the socketed, exsolved nanoparticles on the surface can be specifically tuned to fit the requirements needed for any reaction. [1], [2] A deep understanding of the impact of the elements used for building the perovskite structure are of crucial importance for an intelligent design of perovskite-based catalysts. Therefore, several perovskite-typed oxides, with varying A- and B-site elements were examined in this study. We focused on two points in particular. One, the influence of the chosen elements for the A- and B-site on the capability of catalysing the reaction of **M**ethanol **S**team **R**eforming (MSR). Second, the impact of varying concentrations of B-site dopants (e.g. Cu) on particle growth and formation of the exsolved nanoparticles. For this, *operando* **X**-**R**ay **D**iffraction (XRD) were performed at DESY (***D**eutsches **E**lektronen **Sy**nchrotron*) Beamline P02.1 combined with **S**canning **E**lectron **M**icroscopy (SEM) as well as catalytic test measurements in a fixed bed reactor. The experiments revealed that all investigated materials displayed catalytic behaviour towards MSR. However, we were able to demonstrate that the observed catalytic activity was highly dependent on the elements used for the A-site as well as the concentration of the B-site dopants. Furthermore, the impact of the Cu-content used for the B-site on the formation of nanoparticles could also be proven.

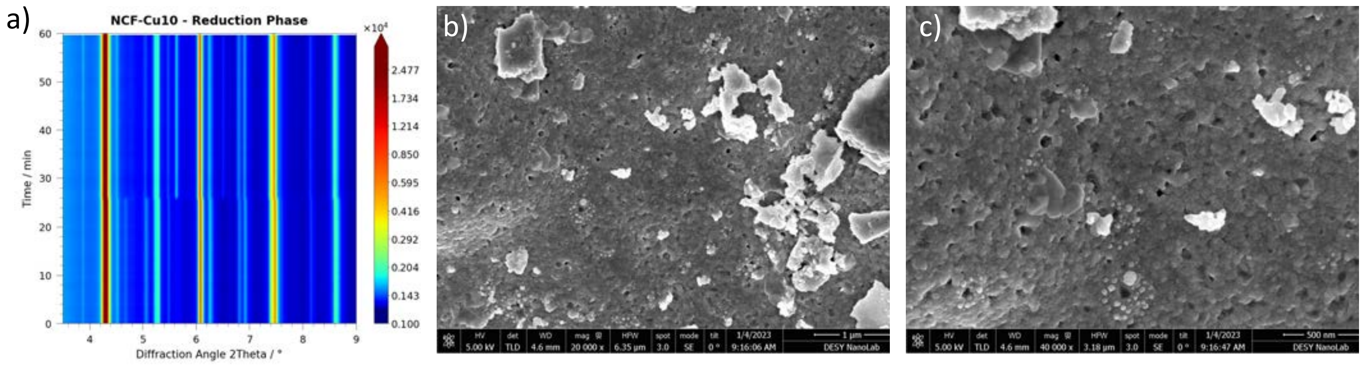

Fig. 1 a) Operando XRD measurement during reducing conditions at Beamline P02.1 at DESY (Hamburg) for $Nd_{0.6}Ca_{0.4}Fe_{0.9}Cu_{0.1}O_3$. Formation of metallic Cu after 25 minutes under reducing conditions. b) and c) SEM images of $Nd_{0.6}Ca_{0.4}Fe_{0.9}Cu_{0.1}O_3$ after reaction conditions of methanol steam reforming proving the formation of nanoparticles on the surface of the material.

[1] D. Neagu *et al.*, *Nat. Commun.*, vol. 6, no. 1, p. 8120, **2015**
[2] L. Lindenthal *et al.*, *Catalysts*, vol. 10, no. 3, Art. no. 3 , **2020**