Structure and dynamics of SCALMS catalysts studied by X-ray and neutron scattering

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Catalysts based on liquid metals offer several advantages, including low toxicity, improved performance, higher selectivity, resistance to coking, and the ability to remain liquid over a wide temperature range. In Supported Catalytically Active Liquid Metal Solutions (SCALMS), gallium serves as a base matrix in the form of nanoparticle droplets on a porous support, hosting small amounts of catalytically active transition metals. The key active sites for catalysis are individual transition metal atoms at the interface, which emerge at the reaction surface spontaneously through diffusion.

Quasi-elastic neutron scattering (QENS) was employed to investigate the diffusion coefficients of Ga and Ni atoms in Ga/Ni alloys as a function of temperature [1], validating ab-initio molecular dynamics (AIMD) simulations on the picosecond timescale. An astonishingly strong influence of small amounts of Ni (2 at.%) was observed, reducing the diffusion coefficient of the alloy by 2 times compared to pure Ga, with minimal change upon increasing Ni concentration.

X-ray and neutron diffraction experiments during heating and cooling cycles, as well as oxidation and reduction processes, showed that largely oxidized Ga/Ni alloy droplets on a highly porous SiO_2 substrate could be reduced in a flow of 5% H_2 in Ar at 800°C, forming Ga_3Ni_2 intermetallic phase. XRD measurements [2] on Ga_3Rh revealed a new structure with the space group $Cmc2_1$, forming isolated reaction sites at the surface. These isolated sites were found to be active in oxidation with only minor deactivation.

[1] A. Shahzad et al., J. Phys.: Condens. Matter, 2024, 36, 175403, 10.1088/1361-648X/ad1e9f
[2] H. Wittkämper et al., Sci. Rep., 2023, 13, 4458, 10.1038/s41598-023-31157-y