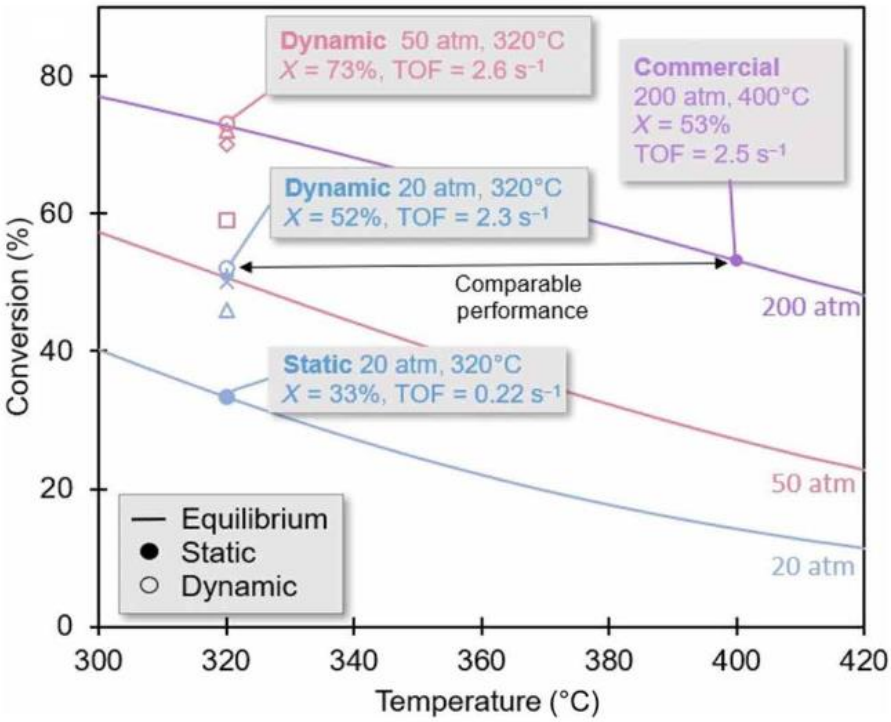
Víctor Sabanza Gil, March 2022

Catalytic resonance of ammonia synthesis by simulated dynamic ruthenium crystal strain

Sci. Adv. **8**, eabl6576 (2022)



Comparison between conversion under industrial conditions, dynamic strain and static strain. Dynamic strain yields similar conversion to industrial reactor but at lower temperature and pressure.

Who are the corresponding authors and what are their research areas?

Paul J. Dauenhauer and Dionisos G. Vlachos. Their main research area concerns the study of catalysts for renewable energy and sustainable economy, with a special remark on the mechanistic understanding of the catalytic processes.

What is the main claim of the article?

The application of dynamic strain to a Ru catalyst in metal-catalyzed ammonia synthesis yields similar conversion to industrial reactors but reduces notably temperature and pressure (from 400 to 320 ºC and from 200 to 20 atm respectively).

Science Advances is a multidisciplinary journal with an impact factor of 14.136 (2021-22). The article is appropriate due to the general-purpose character of the journal and because it shows an interesting phenomenon that could be applied to industry, but only from a theoretical point of view.

How is it demonstrated?

They simulate a solid Ru catalyst under dynamic strain (applied in 2 dimensions) and perform a computational study of surface intermediates and TS involved in NH_3 synthesis using DFT. They observed a shift in metal d-bands that affects adsorbate binding energy and changes rate-determining steps in the reaction.

What are the typical experimental conditions?

DFT calculations are performed using the Vienna Ab initio Simulation Package (VASP) code with the projector augmented wave method. The chosen theoretical conditions are 320 ºC and 20 atm, and the dynamic strain frequencies ranged from 1 kHz to 350 kHz.

Which are the key related papers?

J. Phys. Chem. C **27**, 15500–15505 (2015): DFT study of CO oxidation over a strained Pt surface

ACS Catal. **10**, 12666–12695 (2020): perspective regarding dynamic catalysts and methods to implement surface dynamics

Additional comments, including additional elements of interest

It would be really interesting to experimentally test these conditions to compare with the theoretical predictions. The experimental implementation of the study would require the optimization of the applied dynamic strain.