

## MS42-P07 | A NEW CONCEPT FOR SAPPHIRE SINGLE-CRYSTAL CELLS TO STUDY SOLID-GAS REACTIONS VIA REAL-TIME IN SITU NEUTRON SCATTERING

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Solid-gas reactions get high attention due to far reaching applications, e.g. hydrogen storage, catalysis or the synthesis of functional materials. Revealing reaction pathways and intermediate products by *in situ* neutron diffraction in real-time can help to understand and control such reactions.

Elevated temperature and reactive gases at high pressure require specially designed sample environments. In order to avoid parasitic reflections from the sample holder, sapphire single-crystals are being used. The detection of Bragg reflections of the single crystals can be avoided by proper orientation, resulting in a very low background. Nevertheless, small contributions of the sample holder may still occur due to inelastic scattering from the large crystals, leading usually to the exclusion of about  $5^\circ$  in  $2\theta$  from neutron powder data. Heating is performed contactless by two 100W diode lasers and measured by a pyrometer.

Recent developments are aiming for a reduced mechanical tension between the sample holder and the corpus of the gas pressure cell as well as higher sample temperatures. Therefore, single crystals with reduced wall thickness are used for a better heating efficiency. Further, a newly designed corpus has been developed and tested.

The setup allows to acquire real-time neutron powder diffraction data on solid-gas reactions up to 700 K and 100 bar at the D20 diffractometer (Institute Laue-Langevin, Grenoble). In general, detailed structural information can be extracted by Rietveld analysis with a time resolution in the order of one minute.