Measurement of local crystal lattice strain variations in dealloyed nanoporous gold

Mahr, C.[1], Müller-Caspary, K.[2], Simson, M.[3], Ritz, R.[3], Graf, M.[4], Lackmann, A.[1], Grieb, T.[5], Schowalter, M.[1], Krause, F.F.[1], Mehrtens, T.[1], Wittstock, A.[1], Soltau, H.[3], Weissmüller, J.[4] and Rosenauer, A.[1]

[1] University of Bremen, Germany, [2] EMAT, University of Antwerp, Belgium, [3] PNDetector GmbH, Germany, [4] Hamburg University of Technology, Germany, [5] Universität Bremen, Germany

Application of electric potentials or exposure to gases or liquids causes reversible macroscopic length changes of porous materials such as nanoporous gold (npAu). Thus, these materials are interesting candidates for applications as actuator or sensor. Macroscopic length changes are linked to microscopic changes of crystal lattice parameters. Hence, for the characterisation and improvement of npAu as a functional material measurements of local crystal lattice strain are clearly required. In this contribution we show spatially resolved measurements of crystal lattice strain. NpAu samples have been prepared by corrosion of gold-silver (AuAg) alloys with Ag concentrations of 70at% or 75at% in nitric or perchloric acid. During corrosion Ag is removed from the alloy and Au restructures forming an open porous structure of interconnected gold rich material, the so-called ligaments. Partially these ligaments have a cylindrical form. From continuum theory and atomistic simulation it is expected that cylindrical ligaments show compressive lattice strain along the ligament axis and tensile strain in radial direction[1]. We confirm this expectation by a measurement of local crystal lattice strain variations[2] using a method that is based on nano-beam electron diffraction (NBED) in the scanning mode of a transmission electron microscope (STEM)[3]. Using this method, diffraction patterns are acquired at each scan position of the focussed beam. Distances between spots in the diffraction pattern depend on the local lattice parameter according to Bragg's law. Thus, strain can be determined by measuring distances between diffraction spots in each pattern and comparing them to distances between spots in patterns acquired in a reference region of the sample. For samples without a strain free reference region such as npAu the tetragonal distortion (i.e. the ratio of lattice plane distances in two linearly independent crystallographic directions) is a characteristic measure. We chose axial and radial directions of the cylindrical ligament as the two linearly independent directions to measure the tetragonal distortion. Confirming theory, our measurements show values indicating a compression of lattice parameters along the axis and expansion in radial direction of the ligament. Furthermore, we show the effect of lens aberrations on the measurement of tetragonal distortions and how this effect can be corrected[4]. The strain state of free standing surfaces has an influence on how atoms or molecules adsorb and desorb from the surface and hence on the catalytic activity of the sample[5,6]. Density functional theory predicts predominantly inward relaxation for the majority of flat Au surfaces[7]. Our atomically resolved measurements of strain variations reveal inward relaxation of curved npAu surfaces confirming this theoretical prediction. [1] J. Weissmüller et al., Acta Mater., **58** (2010), p.1.

[2] C. Mahr et al., Mater. Res. Lett., **6** (2018), p.84.

[3] K. Müller et al., Microsc. Microanal. **18** (2012), p.995.

[4] C. Mahr et al., submitted to Ultramicroscopy

[5] M. Mavrikakis et al., Catal. Lett., **64** (2000), p.101.

[6] Q. Deng et al., J. Catal., **309** (2014), p.351.

[7] L. Guan et al., Solid State Commun., **149** (2009), p.1561.

This work was supported by the Deutsche Forschungsgemeinschaft (DFG) within the research unit FOR2213 (www.nagocat.de) and under contracts no. RO2057/11-1 and MU3660/1-1