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Mosaic-like catalysts studied at the Synchrotron MAX IV

Interest in polycrystals has grown significantly in recent years. But what really are polycrystals? Imagine you have a tree trunk and you want to cut planks to build a table. Depending on the angle at which you cut the trunk, the planks will have different patterns. For instance, if you cut the trunk horizontally, the planks will have rings, and if you cut it vertically, they will have stripes. If you cut the tree at some random angle, you will have a pattern somewhere between rings and stripes. Now, let's apply this analogy to crystals. The planks with different patterns in the tree analogy are analogous to single crystal surfaces with different crystallographic orientations. Now imagine, you cannot decide which pattern to choose, you may decide to cut multiple planks at different angles and piece them together to create a table with a mosaic pattern. Similarly, a polycrystal is a crystal that has different parts, called grains with different crystallographic orientations. But what do we need crystals or in this case polycrystals for? The polycrystal used in my thesis is made out of palladium and acts as a catalyst. Catalysts are materials that help to make the conversion process of one gas to another easier. For example, catalysts are used in nearly every car to reduce the amount of emitted exhaust gases and thus reducing global warming.

Coming back to the analogy, since you are now already cutting wood you decide that you need new planks for the cladding of your house. But now, you are asking yourself, do all differently cut planks have the same resistance to the environment? The first thought would be to just test how the planks would react when you observe them while you have, for example, constant rain. But this is not really close to the actual conditions. In reality, the planks will get wet, then they will dry again. They will need to resist low temperatures and snow in winter and also the hot, dry summer weather. So to construct a more realistic experiment, you decide to leave the planks out for multiple years in your garden to observe the changes. But unfortunately, you don't have enough space in your garden to lay out so many differently cut planks. So, you are thinking back to the mosaic-like table that you built earlier and decide just to cut a small part of each different pattern and put them together. Now you have saved a lot of space, and due to the more compact size, you can study all different cuts of wood under the same conditions. To bring the analogy back to my experiment, this is exactly why polycrystals are so useful. They enable comparing measurements of different crystallographic orientations under the same conditions. As for the planks, you will get the most realistic results when you are observing them throughout multiple seasons, meaning you are making constant observations under changing conditions. The same approach is used in the study of catalysis. By taking constant measurements under changing conditions, we can better understand what is happening on the surface and how it affects the efficiency of different grains of catalyst. Unlike the wood experiment, the differences on a catalyst surface cannot be seen with the naked eye. Advanced techniques are needed to study the surface of the catalyst. One of these advanced techniques is ambient pressure x-ray photoelectron spectroscopy, which utilizes x-rays to study what is happening on the polycrystalline surface. In my thesis, I am going to show that ambient pressure x-ray photoelectron spectroscopy can be used to study the single grains of a polycrystal individually. During my thesis, I

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was able to show that temperature-dependent differences of the different grains of the polycrystalline catalyst can be found, which potentially could influence their efficiency.

My thesis demonstrates that ambient pressure x-ray photoelectron spectroscopy can be used effectively to study the individual grains of polycrystals under identical conditions. This opens the way to study more complex reactions on various polycrystalline catalyst materials. This is an important step to gain a deeper understanding of the working mechanism of catalysts. This understanding is crucial for developing new, more efficient catalysis, which is essential for reducing emissions and enabling new technologies for a more sustainable future.

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