Simulating Atomic Dynamics of Pt Nanoparticles on CeO_2 Catalysts

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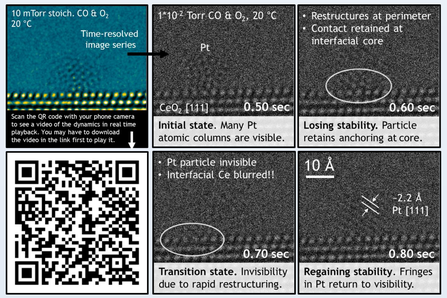
Studying TEM Images of Pt NPs

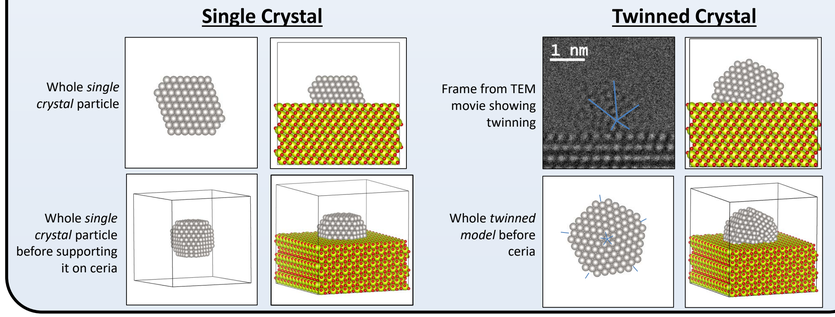
Heterogeneous catalysts play a critical role in chemical conversion processes that impact many societal areas, such as the **Pt NP on CeO_2 system** used in car catalytic converters. Transmission electron microscopy (**TEM**) movies of **Pt NPs in CO & O_2 gas** is one example to study the catalytic structure, to allow later investigation on the structure's affect on functionality. To **determine the average structure (average atomic locations)** in the Pt NPs**,** frames from TEM movies are combined to create a single *summed image.*



Can we determine what is happening to Pt in CO & O_2 and apply this method to other situations?

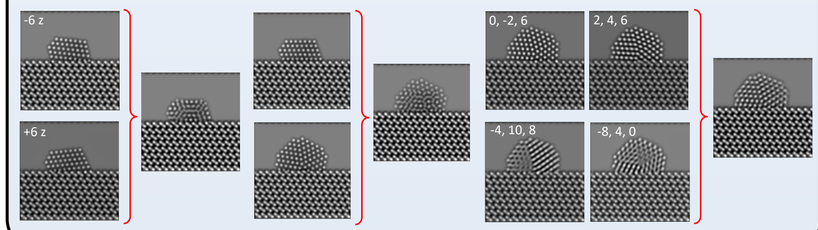
Single vs. Twinned Crystals

Pt is believed to have a single crystal structure in the experimental TEM images because of the visible repeated planes. However, some frames of Pt in CO & O_2 show **twin planes (see image with blue lines). Twinning** occurs when the planes on each side of the grain boundary mirror each other.



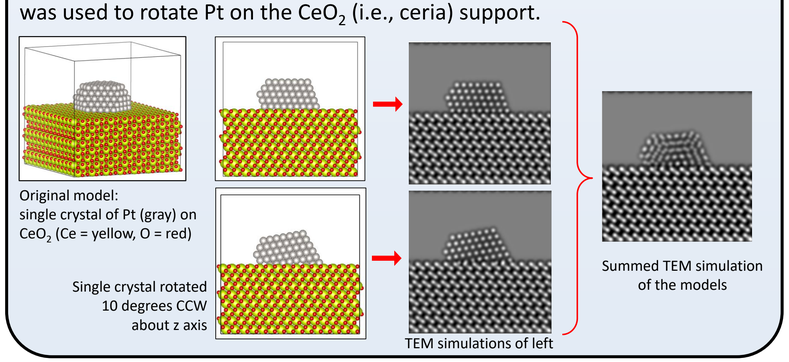
Further Modeling

The spring semester of FURI will bring more analysis to understand how the simulations create different results when summed and **how the rotations and crystallinity affect the summed (or average) image**.



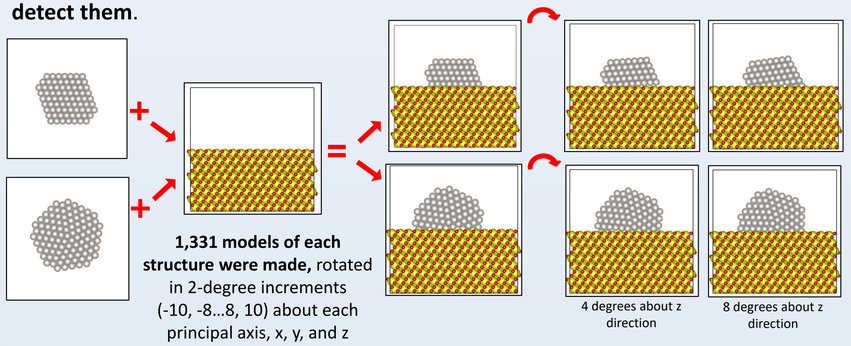
Simulating Structural Dynamics from Static TEM Images

Two **structures of Pt were created** and **rotated about the x, y, and z axes**. Then, **TEM simulations of each rotated structure** were created, attempting to emulate the **structures that could be forming experimentally**. Wulffpack and Rhodius were used to create the structures while Python (Pymatgen) was used to rotate Pt on the CeO_2 (i.e., ceria) support.



Generating Large Sets of Structures Varying in Rotation

A script rotated the spherical particles about the x, y, and z axes, and then **cut off the Pt atoms embedded in the ceria** (not visible in the below images). These **are ideal arrangements** meant to test this method and to determine if these rotations might be happening experimentally; the atoms could be **reconfiguring faster than the TEM can detect them**.



Conclusions

- **Pt NP on ceria in CO and O_2 gas** environment rapidly reconfigures itself. These reconfigurations are visible in TEM movies.
- **It is possible to simulate atomic dynamics through this image-based simulation method.** Further analysis of this is necessary.
- Several structures and different versions of each structure were made to simulate the possibilities, which were **then summed into a simulated TEM images**.
- Understanding these dynamics is important for clean energy materials.

Acknowledgements

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