

ESRP LTHS: Pirates of the Pd Islands: A Study of Nanostructure and Catalytic Functionalities

Atomic-Scale Exploration of Heterogeneous Catalysts

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ABSTRACT

The development of high-performance, cost-effective catalysts is essential to address rising global energy demands and the increasing scarcity of traditional catalytic materials. Functionalized nanocatalysts represent a promising path for overcoming these challenges. While traditional catalytic converters use a full layer of precious metals as a catalyst, prior research suggests that there may be a more efficient distribution.

In this study, we evaluated the structure and functionality of the Pd islands, a specific nanoscale structure consisting of Pd islands on a substrate of Ag(111), as a catalyst for the oxidation of CO. Pd islands were synthesized on a clean Ag surface using physical vapor deposition (PVD) technique. Subsequently, we verified the coverage and structure of the islands via a low-temperature scanning tunneling microscopy (LT-STM). After, we introduced successive treatments of CO and O₂ to the sample and assessed the makeup of the resultant gases using a temperature programmed desorption (TPD) technique. Ultimately, we found that the sample with Pd islands was more effective at oxidizing CO than the sample of only the substrate Ag(111).

BACKGROUND

We are interested in the heterogeneous catalyst Pd/Ag because of its ability to produce many active sites in single atom catalysts and is tolerant to CO poisoning, making it an exceptionally efficient catalyzing material.

The relationship between Pd island formation characteristics (growth, rate, shape) and environmental factors (temperature, pressure, monolayer coverage) has been previously studied, establishing that environmental conditions control how Pd islands form and evolve.

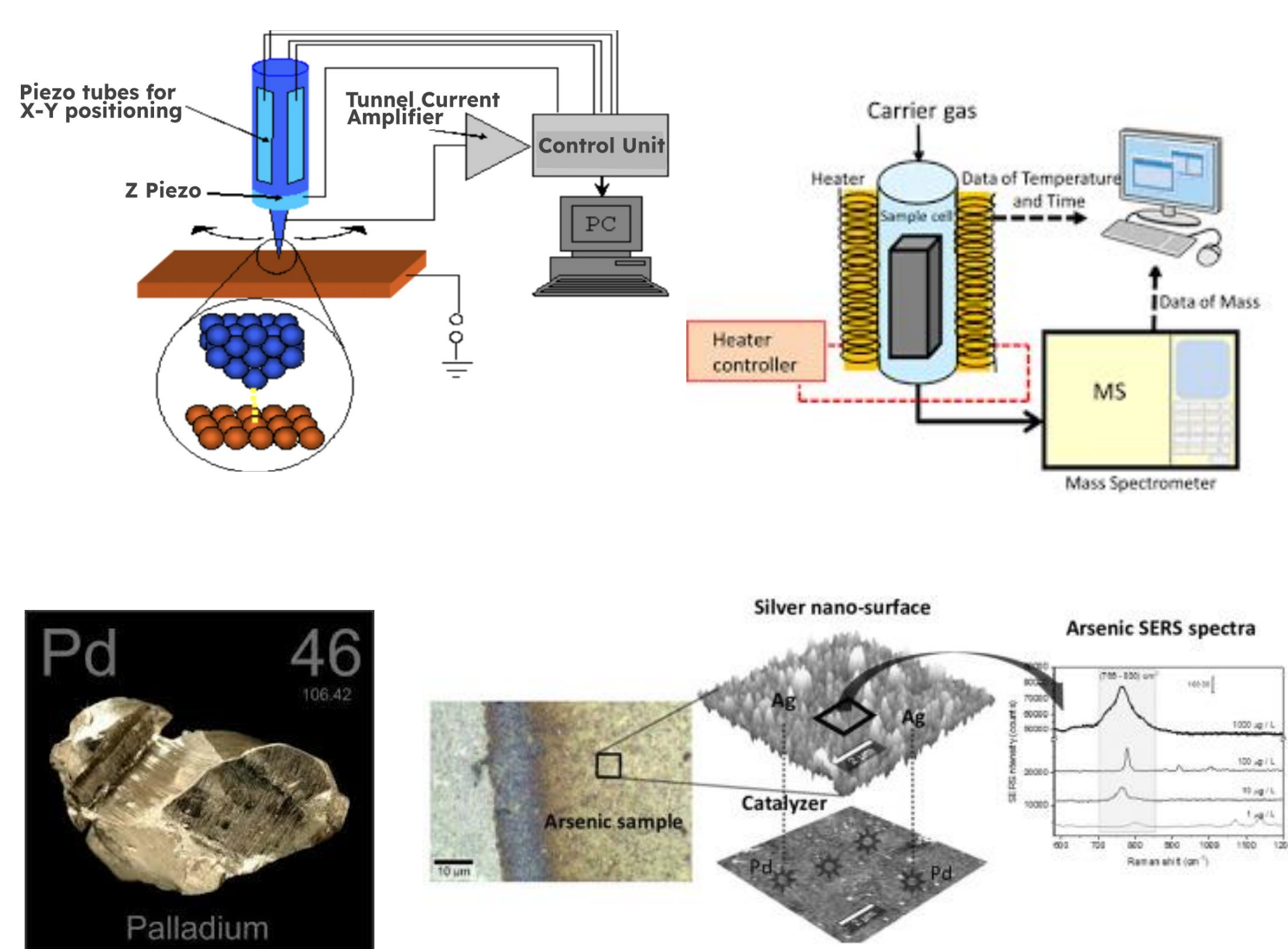
MOTIVATION

The main goal of this study was to improve the resource efficiency of Pd-based catalysts. If the amount of Pd metal in a catalyst is reduced, then the cost of a catalyst will decrease. Cheaper, more efficient catalysts, allow for higher conversion rates and greater selectivity, producing less waste and reducing the need for expensive purification steps.

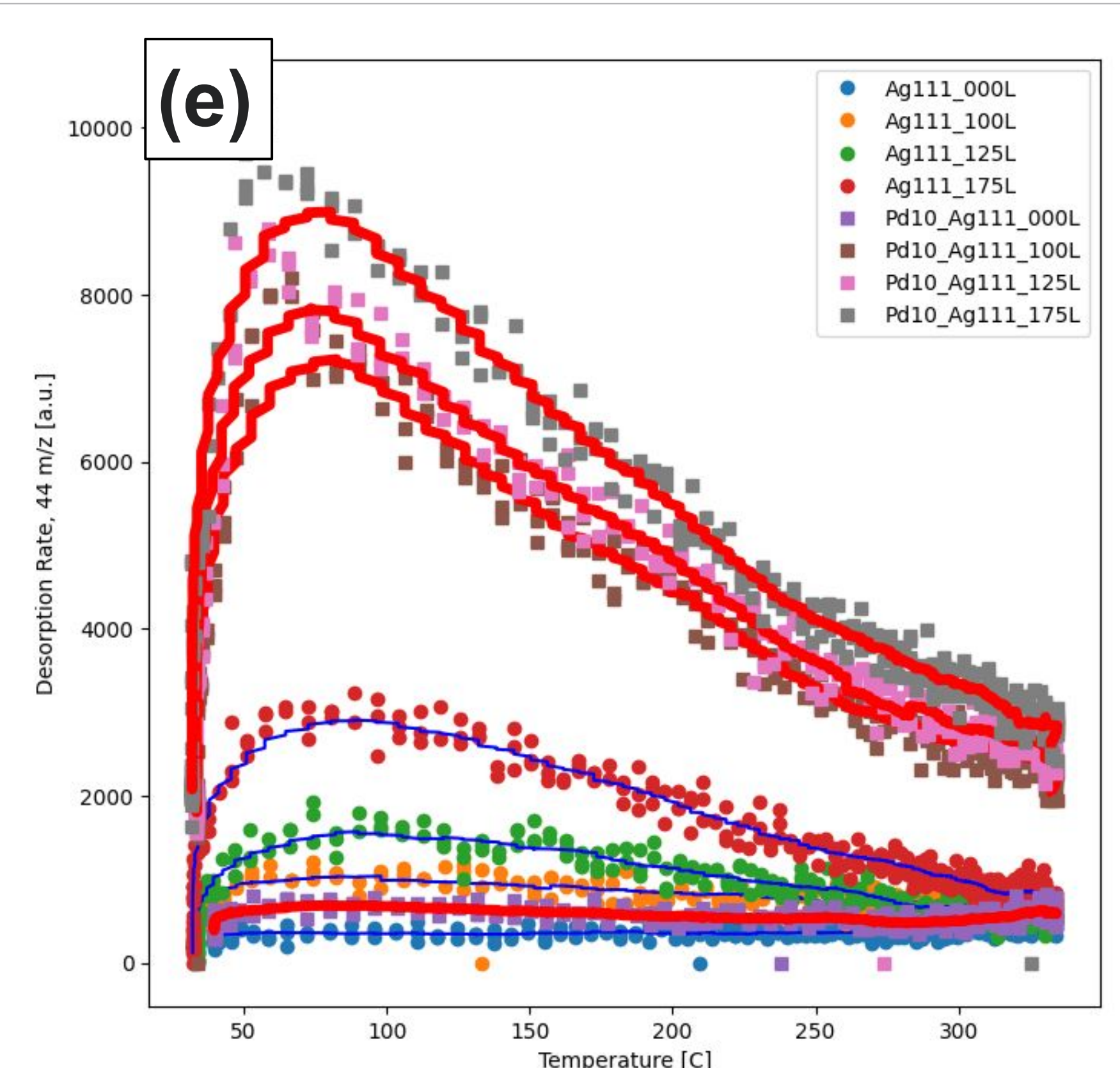
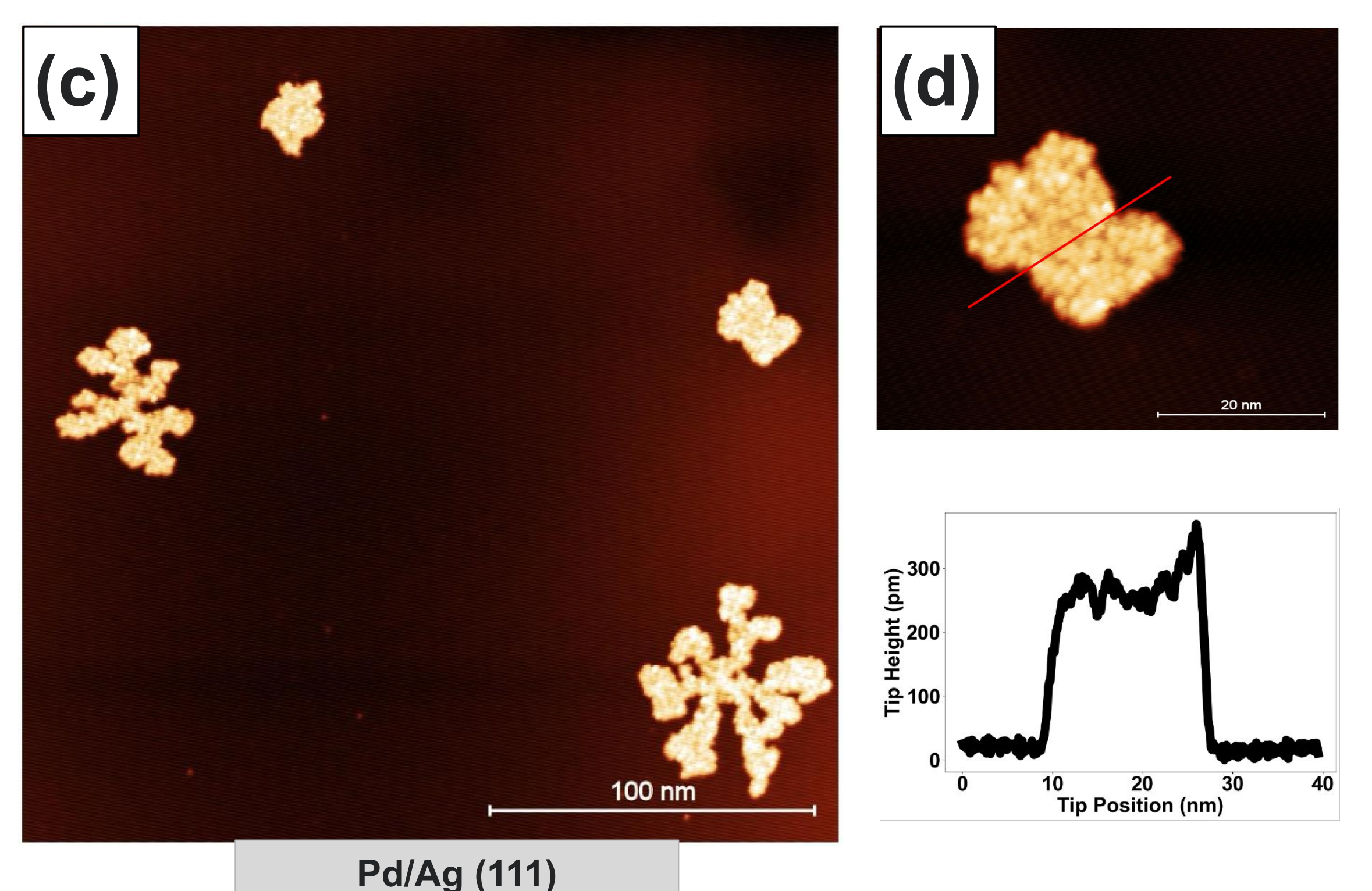
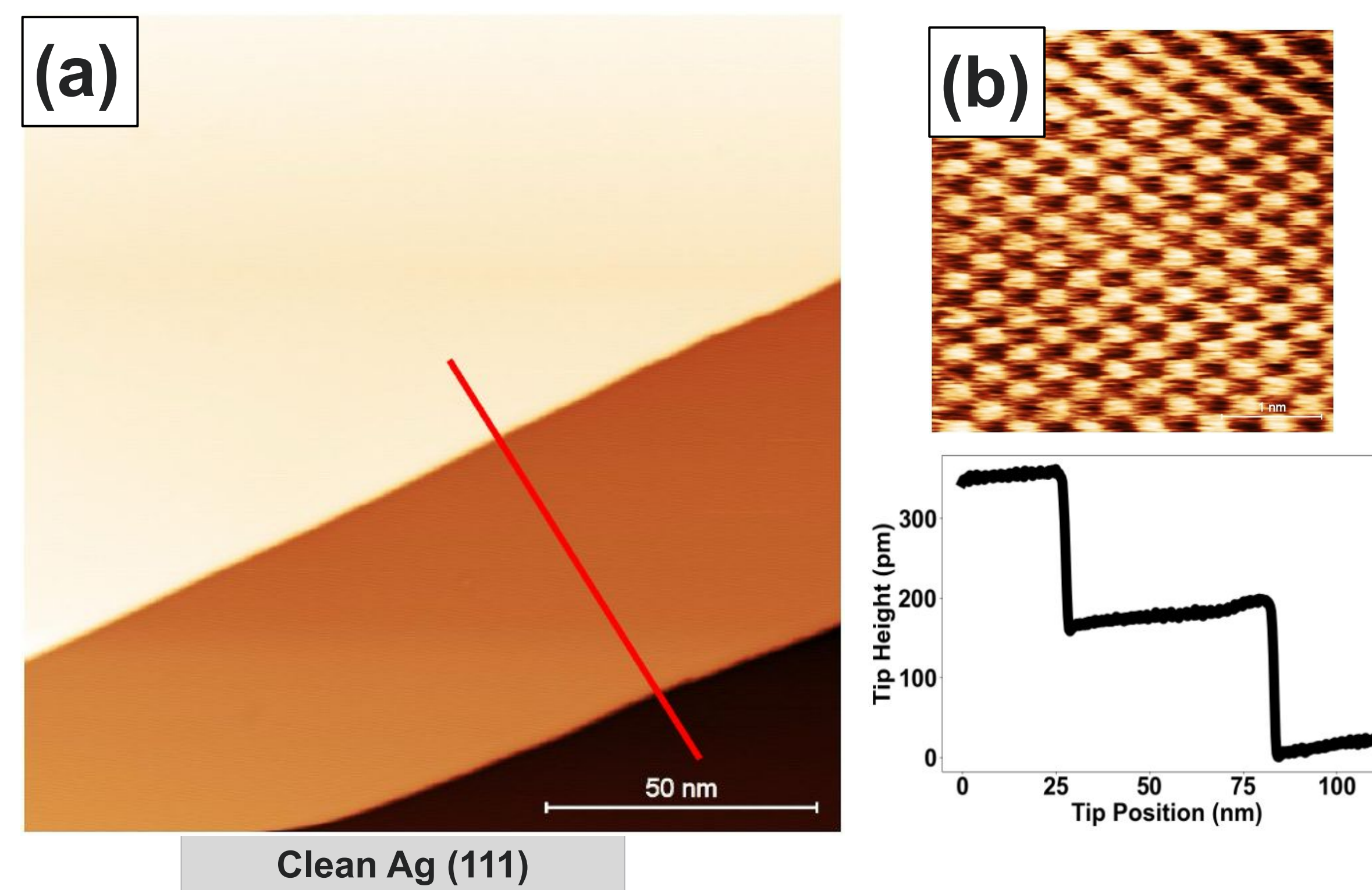
In a broader context, this study advances a worldwide initiative to enhance the economic viability of green technologies.

Method

- Low-temperature scanning tunneling microscopy (LT-STM) and temperature programmed desorption (TPD) techniques
- Argon ion sputtering to clean surface
- Deposited palladium onto silver surface using electron beam physical vapor deposition
 - Measured filament, emission, and flux
- Used scanning tunneling microscopy (STM) to take images
- TPD analyzed surface interactions, specifically adsorption and desorption processes



Data Results



- STM topography images of (a) Ag(111) and (c) Pd/Ag(111). From Ag(111) topography image, atomically clean Ag(111) is successfully prepared. (b) Atomic-resolution Ag(111) image is shown. Based on Pd/Ag topography image, Pd has 0.12 ML (mono-layer) coverage over Ag(111)
- TPD desorption profile of CO₂ (44 amu) on Ag(111) (blue) and Pd/Ag(111) (red line). Average desorption peaks for Ag and Pd/Ag are at 78.7 °C and 86.1 °C, respectively.
- By comparing area under each curve, initial coverage of molecules can be estimated. Compared to Ag and Pd/Ag, initial coverage increases by +250% for 100L.

CONCLUSIONS

- Peak desorption of PdAg at 86.1 °C qualifies desorption may peak at lower temperatures compared to the previously accepted range of 120-130 °C.
- STM imaging confirms island size and geometry expands and complicates as Pd coverage increases, and reveals Pd monolayer island creation may not be strictly hexagonal (Gedara et al).
- Positive correlation between greater Pd coverage and greater maximum desorption, alongside STM topography imaging contributes to existing theory that increased presence of stronger threefold Pd site geometry leads to greater desorption.

NEXT STEPS

- Perform a similar experiment using various amounts of Pd cover on the Ag(111).
- Test different Pd sizes, shapes and surface coverages to determine the structure that has the most efficient catalytic reaction of CO oxidation.
- Compare Pd islands on Ag(111) with other substrate materials to determine how the metal impacts catalytic activity.
- Study long-term stability and durability of Pd islands through repeated trials to determine their practicality in real-world applications.

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