Posudek práce

předložené na Matematicko-fyzikální fakultě
Univerzity Karlovy

❑ posudek vedoucího ☒ posudek oponenta
☒ bakalářské práce ❑ diplomové práce

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Název práce: **Interaction of water vapor with epitaxial layers of cerium dioxide**
Studijní program a obor: **Physics, General Physics**
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Jméno a tituly ~~vedoucího~~/oponenta: **Jesús Rubén López-Roso Redondo**
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Odborná úroveň práce:
☒ vynikající ❑ velmi dobrá ❑ průměrná ❑ podprůměrná ❑ nevyhovující

Věcné chyby:
☒ téměř žádné ❑ vzhledem k rozsahu přiměřený počet ❑ méně podstatné četné ❑ závažné

Výsledky:
☒ originální ❑ původní i převzaté ❑ netriviální kompilace ❑ citované z literatury ❑ opsané

Rozsah práce:
☒ veliký ❑ standardní ❑ dostatečný ❑ nedostatečný

Grafická, jazyková a formální úroveň:
❑ vynikající ☒ velmi dobrá ❑ průměrná ❑ podprůměrná ❑ nevyhovující

Tiskové chyby:
☒ téměř žádné ❑ vzhledem k rozsahu a tématu přiměřený počet ❑ četné

Celková úroveň práce:
☒ vynikající ❑ velmi dobrá ❑ průměrná ❑ podprůměrná ❑ nevyhovující

Slovní vyjádření, komentáře a připomínky vedoucího/oponenta:

This Bachelor thesis is an original, well-designed, and executed scientific work on the interaction of water vapour with cerium oxide (CeO_2) surfaces. CeO_2 is a material widely investigated in fields such as nanomedicine (in the form of nanoparticles) and electrochemistry. The results from this thesis shed light into the water dissociation and surface hydroxylation processes on different CeO_2 surfaces with increased step density. The author conducted and extensive investigation on the preparation of CeO_2 films on Pt(111) in ultra-high vacuum (UHV) with different morphology, and a systematic study of the effect of water vapour exposure on each of them.

In the Introduction, the author makes a compelling argument regarding the importance of the main characterization technique of this thesis: Near-ambient pressure X-ray photoelectron spectroscopy (NAP-XPS). This technique allows the author to investigate the hydroxylation of CeO_2 under realistic conditions that cannot be accessed by traditional UHV-XPS. The material studied and the importance of its surface morphology is also well-described. The hydroxylation of CeO_2(111) is a relatively unfavourable process which still it is known to occur, and drives the redox properties of CeO_2. This hydroxylation is proposed to initially occur at defect sites, such as step edges. The investigation of surfaces which different step edge density is then an excellent approach to gain fundamental knowledge about this phenomenon.

The author makes a proper description of the characterization techniques and step density calculation in the Experimental methods section. The techniques include: XPS, NAP-XPS, low-energy electron diffraction (LEED), quadrupole mass spectrometry (QMS) and scanning tunnelling microscopy (STM). The actual experimental setup is also described in its corresponding section. The experimental work was conducted at the NAP-XPS set-up of the Nanomaterials group at the Faculty of Mathematics and Physics of Charles University. The author shows a fine knowledge of the operation of UHV instrumentation and the solid-state theory and physical principles behind their functioning.

The Experimental results section is separated in (CeO_2) layer preparation and water interaction with the layers. The layer preparation procedures are an extension of previous research by F. Dvořák and T. Duchoň et al. The author shows the ability to understand and reproduce previous literature and build knowledge upon it. The author also reveals a clear understanding of the information that each technique provides: STM for surface morphology, XPS for chemical identification and layer thickness, and LEED for the crystalline structure. The film preparation required thorough substrate cleaning and precise Ce-deposition/thermal treatment. Each film, named *classical layer*, *gradual layer*, and *redox layer*, requires different growth parameters which are properly addressed in the text. The author does not only describe these parameters but demonstrates a complete understanding of the role of the growing conditions (e.g.: *[…]the heating and cooling process should be slow, otherwise, the CeO_2 layer could crack due to the fact that the two different layers have different reactions to heat, […])*. The interaction of the layers with water is investigated by in-situ NAP-XPS measurements at elevated water pressure (up to 1mbar). The author produces a concise description of the NAP cell cleaning procedure and water dozer preparation, which is essential to ensure the quality and reproducibility of results. All the experimental parameters (sample temperature, water pressure, X-ray exposure time) used for the investigations of the water effect on each layer are well-described. The comparison of the O 1s and Ce 3d lineshapes for each exposure and layer provides the key fingerprints to identify the hydroxylation threshold of the surfaces, and demonstrates that the hydroxylation is promoted at step edges rather than on terrace sites. Moreover, a certain degree of Ce^{4+} to $Ce3^{+}$ reduction is observed.

To summarize, the author of this bachelor thesis demonstrates an overall excellent knowledge of the fundamentals and capabilities of UHV and surface science. The author provides proper credit to previous research and is able to inform the reader about the soundness of the research conducted for the thesis. The author describes the experimental conditions in a clear way which allows reproducibility and demonstrates a systematic and well-planned approach to this kind of UHV investigations. This is a high-quality and scientifically sounding thesis, which I recommend as *vynikající.*

Případné otázky při obhajobě a náměty do diskuze:

1) The NAP-XPS machine shown in Figure 3.1 has a monochromator which is not mentioned in the description of the machine. What is its purpose? How does it influences the XPS measurements?
2) The author mentions earlier works of CeO_2 layer growth on Cu. Why is Pt chosen as the substrate for CeO_2?
3) Is there any shift/different components between the Pt 4f lineshape of the three CeO_2 films?
4) If there was no STM available, XPS could be use to infer whether the CeO_2 is a closed film or there are patches of bare Pt. How would you measure it?

Práci
☒ doporučuji
❑ nedoporučuji
uznat jako diplomovou/bakalářskou.

Navrhuji hodnocení stupněm:
☒ výborně ❑ velmi dobře ❑ dobře ❑ neprospěl/a

Místo, datum a podpis vedoucího/oponenta:

V San Sebastián, 13/06/2023

Jesús Rubén López-roso Redondo