Epitaxizing Untwinned $PdCoO_2$ Films by MBE

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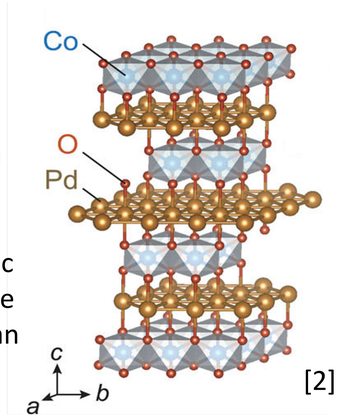
Introduction

Delafossite—$PdCoO_2$

- Delafossite materials have a layered **triangular** structure with chemical formula ABO_2.
- $PdCoO_2$ is one of the metallic delafossites with high in-plane **conductivity**, even higher than pure Pd metal [1].

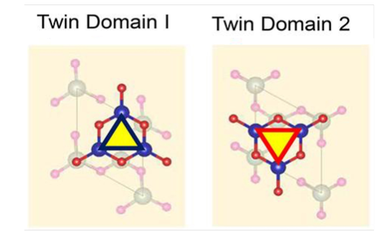


[2]

Research Question

Growing by MBE, structural defects contribute to higher resistivity. On **Al_2O_3 (0001)** substrates, the crystal structure in each one-monolayer-high step face in a different direction alternately, resulting in $PdCoO_2$ growing on top of them having triangular structures 180º opposite from each other, called "**twinning**".

To solve twinning, Al_2O_3 substrates are made to have steps with **two-monolayer heights**, all facing in the same direction. We hope $PdCoO_2$ grown on top will have triangles in the same direction, thus achieving untwinned films.



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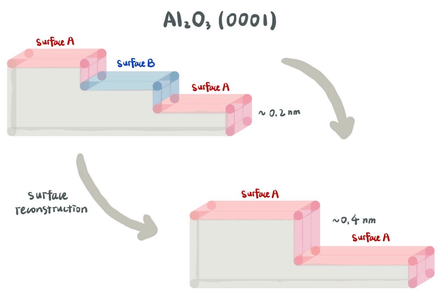


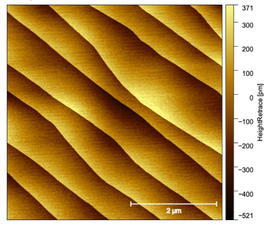
Methods

Specially treated Al_2O_3 substrates are provided by our collaborators. We use Molecular Beam Epitaxy (MBE) for absorption control growth, monitored by RHEED. After-growth characterizations include XRR, XRD, ϕ-scan, and AFM. ϕ-scan (6 peaks instead of 3 show twinning) and AFM are especially important for twinning analysis.

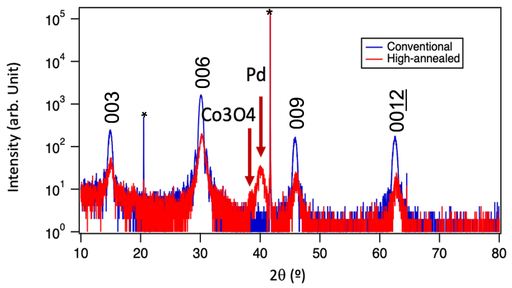
Results

One specially treated Al_2O_3 substrate was scanned with AFM before growth. Step height measured was around 0.449 nm, which is two monolayers.

Special Al_2O_3 substrate

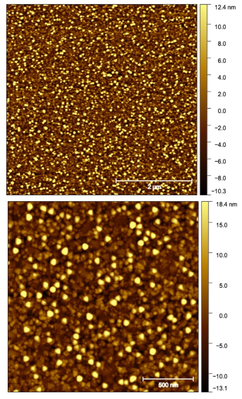


Same growth conditions on regular and special Al_2O_3



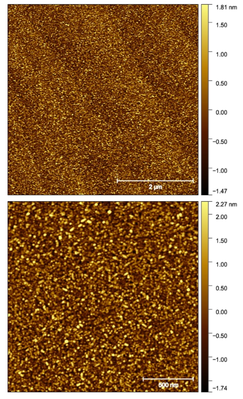
With same growth conditions for regular substrates on special substrates, **impurities** appeared (E.g., Pd and Co_3O_4). Surface energy of substrate changed. New growth conditions are required.

Pd Impurity

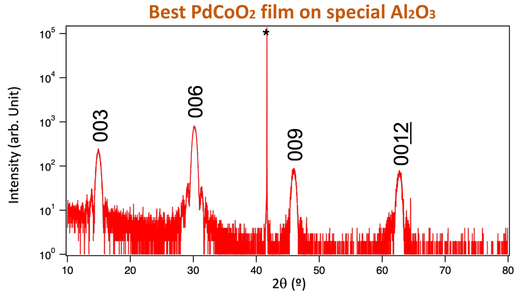


AFM images were taken for different impurities.
Left – big dots of ~30nm high and ~100nm wide – **Pd**.
Right – small dots of ~8nm high and ~60nm wide – **PdO**.

PdO Impurity

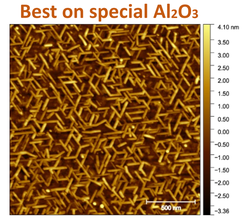


Best $PdCoO_2$ film on special Al_2O_3

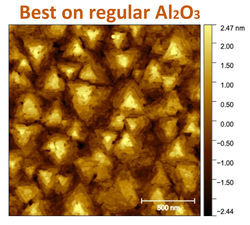


With improvement, we achieved almost **pure** $PdCoO_2$ films. XRD shows strong peaks with fringes. AFM image (top right) shows three-fold strips on the surface,

Best on special Al_2O_3

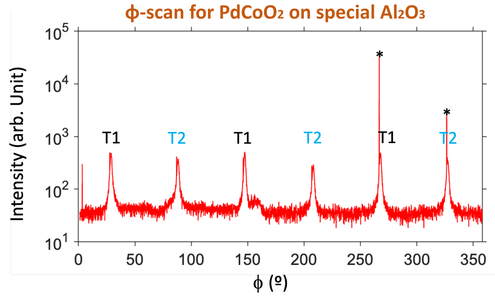


Best on regular Al_2O_3



which is different from triangles we usually see on regular Al_2O_3 substrates (bottom right in middle column).

ϕ-scan for $PdCoO_2$ on special Al_2O_3



For triangular $PdCoO_2$, 6 peaks of equal intensity are presented in ϕ-scan, indicating twinning still exists.

Conclusion

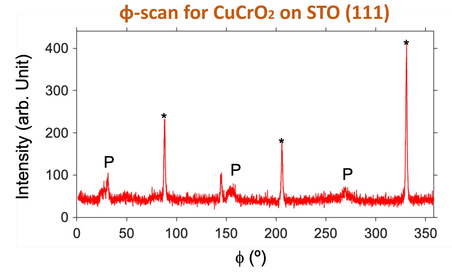
On two-monolayer step height special Al_2O_3 substrates:

- Distinguished various impurity phases in AFM images
- Almost achieved pure $PdCoO_2$
- Haven't solved twinning problem

Future directions:

Grow $PdCoO_2$ on untwinned **$CuCrO_2$** buffer layer to solve twinning problem. See hope as we have successfully grown untwinned $CuCrO_2$ films.

ϕ-scan for $CuCrO_2$ on STO (111)



Acknowledgements

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References

[1] A. P. Mackenzie, "The properties of ultrapure delafossite metals", Rep. Prog. Phys. 80 032501 (2017).
[2] T. Harada, K. Fujiwara and A. Tsukazaki, "Highly conductive $PdCoO_2$ ultrathin films for transparent electrodes", APL Mater. 6, 046107 (2018).
[3] J. M. Ok, et al., "Twin-Domain Formation in Epitaxial Triangular Lattice Delafossites", ACS Appl. Mater. Interfaces 13, 22059−22064 (2021).

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