Abstract Submitted
for the NWS17 Meeting of
The American Physical Society

The effect of amorphous precursors on the crystallinity of TiO_2 thin films using Pulsed Laser Deposition[1] JAMES HAGGERTY, Oregon State University, LAURA SCHELHAS, SSRL, JOHN MANGUM, CSM, LAUREN GARTEN, NREL, DANIIL KITCHAEV, MIT, WENHAO SUN, LBNL, OKAN AGIRSEVEN, JANET TATE, Oregon State University, MICHAEL TONEY, SSRL, JOHN PERKINS, NREL, BRIAN GORMAN, CSM, GERBRAND CEDER, LBNL, CENTER FOR THE NEXT GENERATION FOR MATERIALS BY DESIGN COLLABORATION — TiO_2 is a well-known transparent metal oxide with three naturally occurring polymorphs, rutile, anatase, and brookite. It is used in many applications ranging from photocatalysis, cosmetics, gas sensors, and the biomedical industry. We aim to understand how the crystallization pathways are affected by the presence of metastable anatase and stable rutile in relation to metastable brookite. We use DFT calculations to explore helper-ion incorporation, substrate matching, and chemical transformations to guide synthesis of brookite thin films. Amorphous thin films are deposited on various substrates by pulsed laser deposition. Structural characterization by X-ray diffraction is performed in-situ during rapid and conventional annealing and reveals the formation of brookite upon heating to 340C. Micro-Raman spectroscopy and atomic force microscopy together map the micron scale regions of pure brookite. TEM is used to examine ion incorporation from the substrate and its contribution to the formation of brookite.

[1]The work was supported as part of the CNGMD, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science

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Date submitted: 05 May 2017 Electronic form version 1.4