Scientists develop data origami approach to find optimal process routes in photovoltaics

One of the challenges in improving the performance of photovoltaic (PV) devices is to correlate device performance characteristics with the various process steps and conditions utilized in synthesizing or manufacturing the completed devices. At the National Renewable Energy Laboratory (NREL), the multivariate features of nature inspired scientists to develop better PV devices by modeling multivariate data ranging from processing histories and assessed material data from various characterizations to the final performance.

NREL researchers adapted the concept of origami, which consists of folding, cutting, and pasting papers, to complex PV data for identifying the effects of process conditions on the final performance of solar devices. Through data origami, data transform to more effectively reveal hidden relationships between process, material properties, and performance of the devices.

NREL researchers uncovered multiple interdependencies between approximately 30 properties and seven growth conditions of the Al-doped ZnO (AZO) layer, which is an essential component of CuInxGa1-xSe2 solar devices. Figure 1 shows the parallel coordinate, a high-dimensional visualization approach, to visualize the numerous correlations of cross-linked variables in data origami-treated AZO datasets for overcoming the curse of dimensionality. The abscissa in parallel coordinates represents each variable, whereas the ordinate represents 10 different levels of variables. For instance, the figure-of-merits at 500 and 550 nm of the AZO films result from the noticeable low values of forward power of sputtering target and process pressure of sputtering chamber, and the increase in mobility and film thickness with decreasing film resistivities.

NREL researchers are also developing virtual metrology based on these correlations, which can correlate, predict, and ultimately control measurable parameters as well as non-measurable theory-based properties.

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Key Research Results

Achievement
NREL researchers are using the principles of origami—folding, cutting, and pasting—to look for multiple variables and aspects of PV materials. Following physics-based theories, they are adding information not directly measurable to the data set to better analyze how optical response, electrical transport property, and other variables can combine to optimize a solar cell’s performance.

Key Result
NREL researchers uncovered multiple interdependencies between approximately 30 properties and seven growth conditions of the aluminum-doped zinc oxide layer, which is an essential component of copper indium gallium selenium solar devices. The derived properties will be useful as virtual characterization tools because they don’t have to be installed in the PV process lines and don’t add any cost.

Potential Impact
PV manufacturers may benefit from the advanced knowledge without any need to retrofit, thereby boosting performance without having to boost prices.