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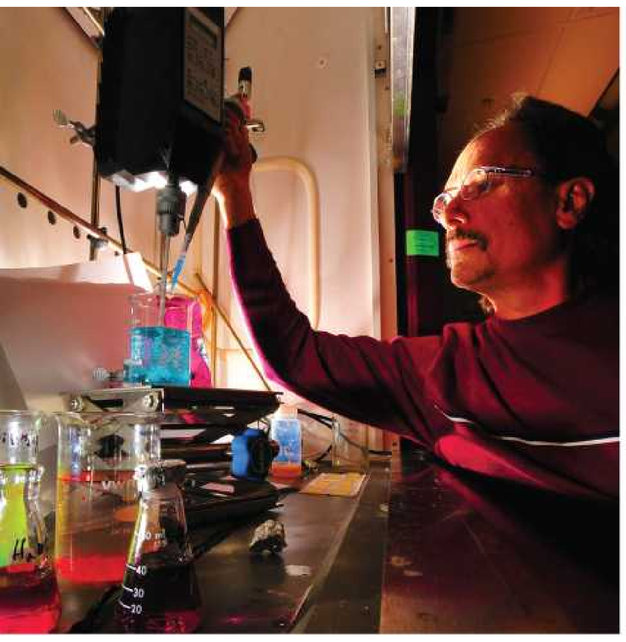
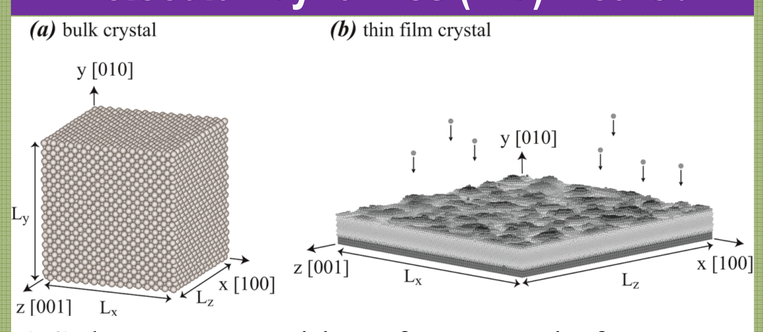


Molecular Dynamics Simulations of Diffusion Induced Aging in PV Modules

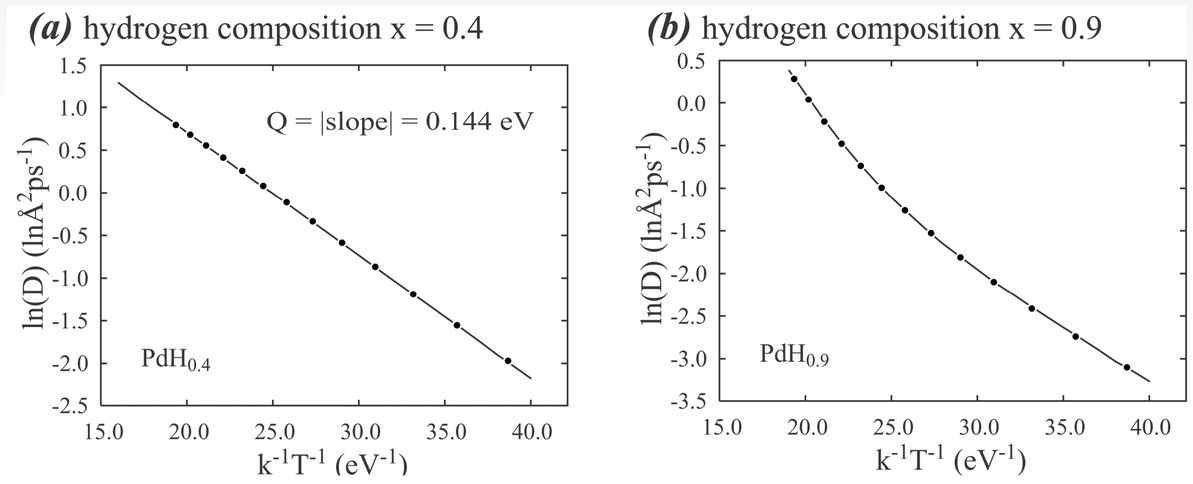
CdTe modules undergo an initial 4-7% degradation over the first 1-3 years and a 0.5-0.7%/year degradation thereafter (Report IEA-PVPS T13-01:2014). While this has been attributed to the grain boundary diffusion of copper from the back contact, progress to reduce this degradation has been slow due to the long cycle of aging experiments. Sandia has developed large scale atomistic simulation methods that approach the accuracy of quantum mechanical calculations (PRB, 85, 115206, 2012; PRB, 86, 245203, 2012; J. Phys. Chem. C; J. Mater. Sci., 50, 2859, 2015). Sandia also developed new algorithms that overcome the time scale of atomistic simulations and at the same time accounts for the statistics of atom diffusion on all lattice sites (J. Phys. Chem. C, 120, 7500, 2016). When leveraged with super computing power, we can study not only copper diffusion on all possible grain boundaries, but also grain boundary evolution under the thermal and mechanical cycles. As a result, our computational studies can be used to design new chemistry and to engineer new grain boundaries that minimize diffusion–induced aging. They can also be used to derive relations that connects experimental aging data obtained under accelerated conditions to real conditions, which will impact a variety of current efforts to improve PV modules.

Molecular Dynamics (MD) Method



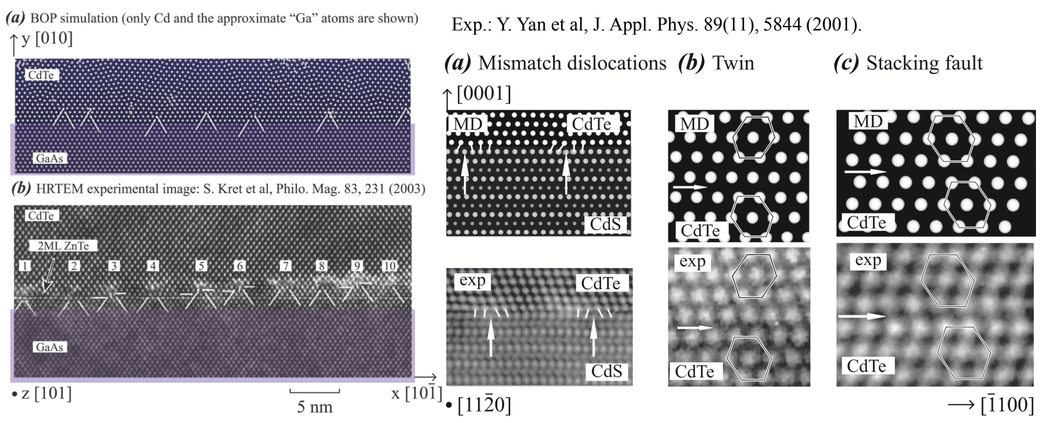
1.Solves atom positions from atomic forces;
2.Predict high-resolution structures accurately.

Diffusion Studies (Palladium Hydride Is Used only as an Example)



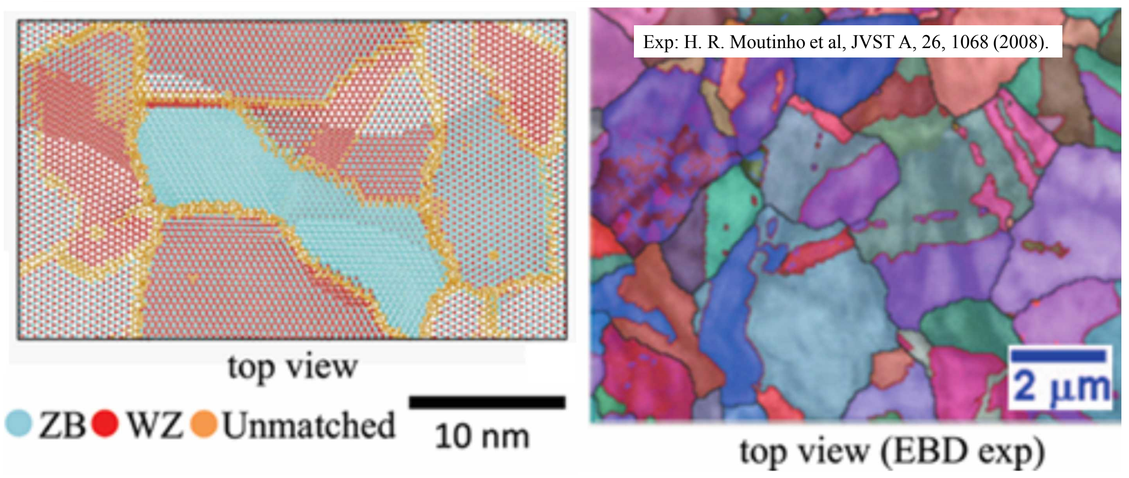
MD statistically account for all atomic jump paths at grain boundaries and yet results in highly converged Arrhenius plots. This is an advantage over quantum mechanical calculations, enabled only by super computing power.

Comparison of MD Prediction and Experiments on High Resolution Microstructures



Without any assumptions other than randomly injecting adatoms on the growth surface, MD simulations reproduce well the experimentally observed high resolution microstructures.

Comparison of MD Prediction and Experiments on Grain Structures



Without any assumptions other than randomly injecting adatoms on the growth surface, MD simulations reproduce well the experimentally observed grain structures.

In the near term, this project will answer such question as how diffusion impact properties of PV modules as a function of time, how PV properties measured from accelerated aging experiments can be accurately converted to those under the operating conditions, and how materials' chemistry and microstructure can be engineered to improve durability. Between 1 and 5 years, the capability can be integrated into production cycle of CdTe PV modules. In five years, this tool may begin to impact other PV modules.

U.S. DEPARTMENT OF ENERGY

National Nuclear Security Administration

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