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Thermal Evolution of Defects and Hydrogenated Surfaces in nc-Si:H

KRISTIN KIRILUK, DON WILLIAMSON, Colorado School of Mines,
DAVID BOBELOA, National Renewable Energy Lab, ARUN MADAN, FENG ZHU,
MV Systems, Inc., P. CRAIG TAYLOR, Colorado School of Mines — Photovoltaics
research has created a push for new materials and nanotechnology is a primary fo-
cus. The most familiar of the nanomaterials is hydrogenated nanocrystalline silicon
(nc-Si:H). nc-Si:H has less light-induced degradation than a-Si:H and is cheaper to
make than crystalline silicon. X-ray diffraction (XRD), small angle X-ray scattering
(SAXS), and electron spin resonance (ESR) experiments explored the crystallite size,
orientation and defect density on nc-Si:H samples with varying crystalline volume
fraction (CVF). Samples with CVF \( \sim \) 50% show preferential [220] crystallite orienta-
tion, whose microstructure changes with thermal annealing. Modeling of SAXS
data for as-grown material shows that the crystallite surfaces are 20% to 40% hydro-
genated. After high temperature annealing, hydrogen leaves these surfaces and the
ESR signal increases by about 10 times. We discuss these results and then speculate
on the relationship between hydrogen, defects, and microstructure.

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Kristin Kiriluk
Colorado School of Mines

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