

# Improving SnS Performance through Targeted Defect Management (PV-4)



A joint India-U.S. research consortium funded under the *Joint Clean Energy Research & Development Center (JCERDC)*

## Scientific Achievement:

We computationally predicted lifetime-limiting point defects in SnS—the sulfur vacancy  $V_S$  and impurity-related substitutionals  $Fe_{Sn}$ ,  $Co_{Sn}$ , and  $Mo_{Sn}$ . We also optimized growth parameters to suppress these defects and achieved  $>1$  ns lifetime in SnS crystal samples.

## Significance and Impact:

Device modeling indicates that  $>1$  ns lifetimes enable  $>10\%$  SnS devices if we can translate this success to thin films. To our knowledge, this is the first-ever  $>1$ -ns lifetimes in SnS. Thus, 1-ns lifetime in SnS constitutes a major advance in the main limiting factor for SnS devices.

## Research Details:

- Predicted defect impact on lifetime with DFT (collaboration with WUSTL through SERIIUS) and Shockley-Read-Hall recombination model.
- Crystal growth from 99.9999%-pure Sn and S.
- Control for sulfur content and metal impurity content.
- Improved minority-carrier lifetime to  $>1$  ns in S-rich, high-purity crystals.
- Close-spaced sublimation furnace has been built to translate these learnings to thin films, with preliminary indications of lifetime improvements over previous thin films.

**Publication(s):** A. Polizzotti, A. Faghaninia, J.R. Poindexter, L. Nienhaus, V. Steinmann, R.L.Z. Hoyer, A. Felten, A. Deyine, N. Mangan, J.P. Correa-Baena, S.S. Shin, S. Jaffer, M. Bawendi, C. Lo, T. Buonassisi, "Improving carrier lifetime of tin sulfide via prediction and mitigation of harmful point defects," *J. Phys. Chem. Letters* **8**(15), (2017).

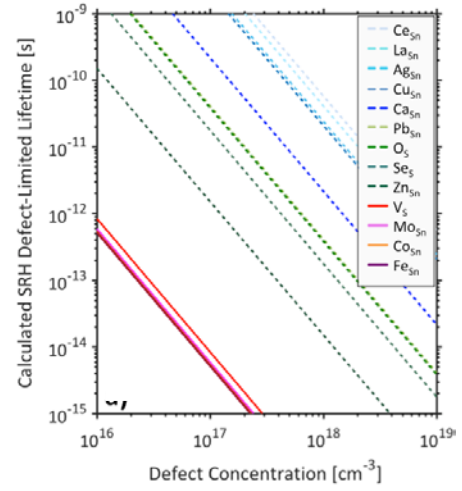


Fig. 1: Predicted defect-limited lifetime for specific defects vs. defect concentration. Even at low concentrations, four defects limit carrier lifetime ( $V_S$ ,  $Mo_{Sn}$ ,  $Co_{Sn}$ ,  $Fe_{Sn}$ )

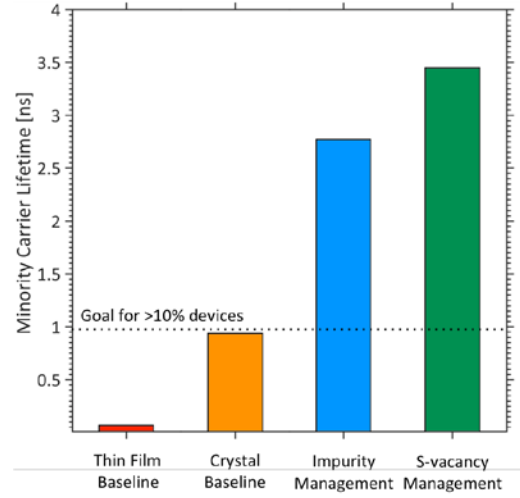


Fig. 2: Lifetime improvements with impurity and sulfur vacancy management. These results enable  $>10\%$  devices if translated to thin films.

**Contact(s):** Tonio Buonassisi ([buonassisi@mit.edu](mailto:buonassisi@mit.edu)) & Alex Polizzotti ([a\\_zotti@mit.edu](mailto:a_zotti@mit.edu))