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

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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.

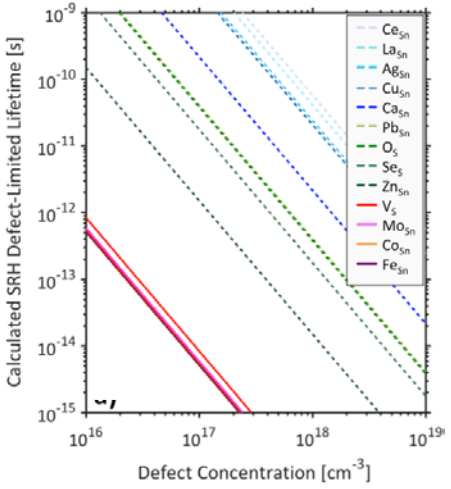

Fig. 1: Predicted defect-limited lifetime for specific defects vs. defect concentration. Even at low concentrations, four defects limit carrier lifetime (V_S, Mo_{Sn}, Co_{Sn}, Fe_{Sn})

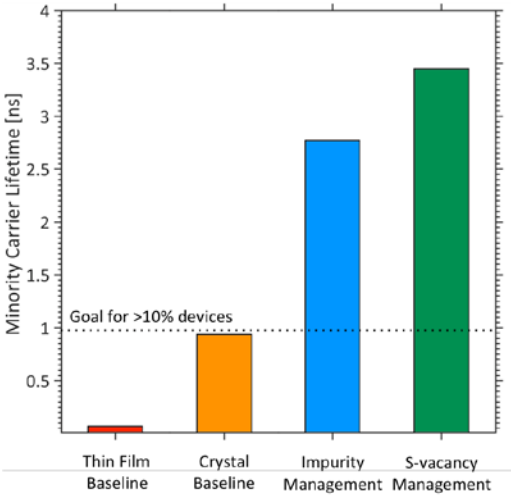

Fig. 2: Lifetime improvements with impurity and sulfur vacancy management. These results enable >10% devices if translated to thin films.

Publication(s): A. Polizzotti, A. Faghaninia, J.R. Poindexter, L. Nienhaus, V. Steinmann, R.L.Z. Hoye, 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).

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