Atom Gazing for Improved Solar Energy

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Introduction

- Solar energy has vast potential for
  - decarbonisation of energy systems
  - broad and equitable electrification
  - carbon neutrality
- 95% of solar panels made from Silicon
  - Abundant, stable, lightweight, and efficient.
- More solar energy deployment requires even more efficient panels.
- Tackling climate change requires Solar energy deployment in the multi-TW/year.

Specimen Details

- SiN$_x$ has hydrogen (H) and deuterium (D).
- H/D released with a 2 min 500°C anneal.
- A very fine needle is made across layers using electron microscopy (red area).

Atom Probe Tomography (APT)

- Needle is cooled to <80K, held at DC electric potential, and blasted with laser pulses.
- Atoms vapourised by the blast are detected by a position sensitive detector.
- The time that it takes for atoms to fly is used to identify what elements they are.

What is the atomic composition of the solar cell nanolayers?

- Ionic species from each element inside the needle are identified on mass spectrum (below).
- The key species are chosen and a digital 3D reconstruction is calculated (right).
- $^{16}$O (blue map) marks the location of oxide and SiN$_x$ (with H inside)
- Mass-to-charge ratio of 4 Da unambiguously attributed to Deuterium – a signature of H presence.
- H accumulates at interfaces to improve performance.

Conclusions

- APT offers 3D digital reconstruction of the atoms that compose interface nanolayers, and allows chemical analysis suitable for the understanding of next generation solar cells.
- Hydrogen is identified at the interfaces, and found to be a crucial element that mediates the effectiveness of the nanolayer sandwich in solar cell operation [3].
- Controlling hydrogen in nanoscale sandwiches has become a major area of materials and process engineering leading to the improvement of solar cell technology.
- Understanding materials at the atom scale will enable technical advances and contribute to the broad deployment of solar energy – a crucial renewable technology for a zero-carbon future.

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