

Semiconducting Metastable Sn₃N₄ and IV₃N₄ Polymorphs

Scientific Achievement

Thin films of the metastable spinel γ -Sn₃N₄ were synthesized by sputtering and characterized for semiconducting properties, such as absorption spectra, electrical transport, ionization potential, and minority-carrier diffusion length.

Significance and Impact

Experiments indicate that Sn₃N₄ would be promising for PEC water oxidation, either by reducing its hole effective mass by alloying with Si/Ge or by stabilizing the α - or β -polymorphs, as suggested by first-principles theoretical calculations.

Research Details

- **Synthesis:** Thin films of metastable γ -Sn₃N₄ (+1.56 eV/f.u.) were synthesized by reactive sputtering with atomic nitrogen.
- **Optical:** The measured optical gap of γ -Sn₃N₄ is 1.6 eV, in good agreement with 1.5 eV theoretical calculations (Fig. 1).
- **Electronic:** The γ -Sn₃N₄ ionization potential is 6.0–6.5 eV, suitable for water oxidation applications (*n*-type, 10¹⁸ cm⁻³).
- **Theory:** Hole effective mass of γ -Sn₃N₄ (13m_e) can be decreased by alloying with Si/Ge, and stabilizing α - or β -polymorphs (Fig. 2).

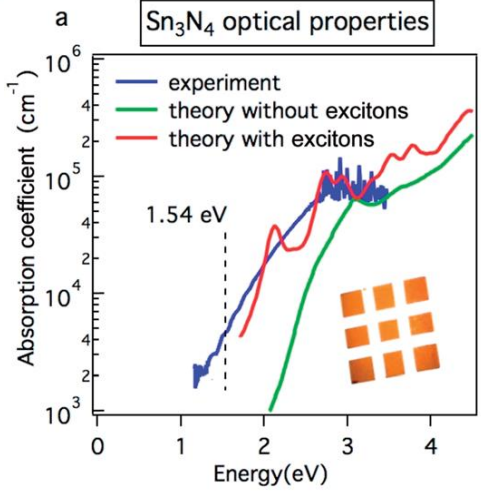


Fig. 1. Optical absorption of Sn₃N₄

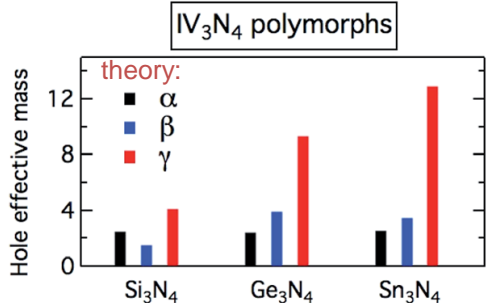


Fig. 2. Hole effective masses of IV₃N₄ polymorphs

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