Semiconducting Metastable Sn_3N_4 and IV_3N_4 Polymorphs

Scientific Achievement

Thin films of the metastable spinel γ-Sn_3N_4 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 Sn_3N_4 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-Sn_3N_4 (+1.56 eV/f.u.) were synthesized by reactive sputtering with atomic nitrogen.

– **Optical:** The measured optical gap of γ-Sn_3N_4 is 1.6 eV, in good agreement with 1.5 eV theoretical calculations (Fig. 1).

– **Electronic**: The γ-Sn_3N_4 ionization potential is 6.0–6.5 eV, suitable for water oxidation applications (*n*-type, 10^{18} cm^{-3}).

– **Theory**: Hole effective mass of γ-Sn_3N_4 ($13m_e$) can be decreased by alloying with Si/Ge, and stabilizing α- or β-polymorphs (Fig. 2).

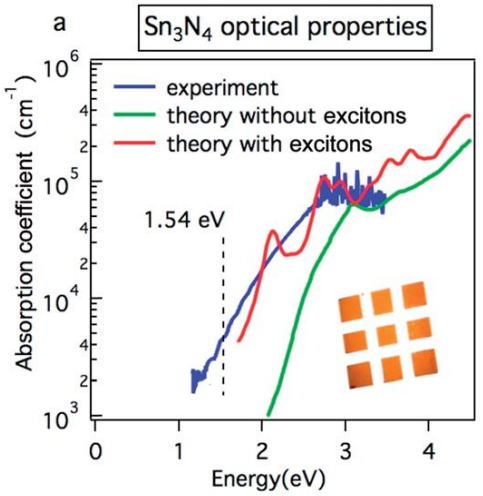

Fig. 1. Optical absorption of Sn_3N_4

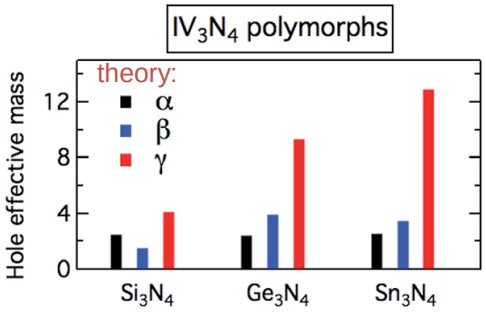

Fig. 2. Hole effective masses of IV_3N_4 polymorphs

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