Silver Vanadates: A New Class of Computationally Designed *p*-type Transparent Conducting Oxides

Scientific Achievement

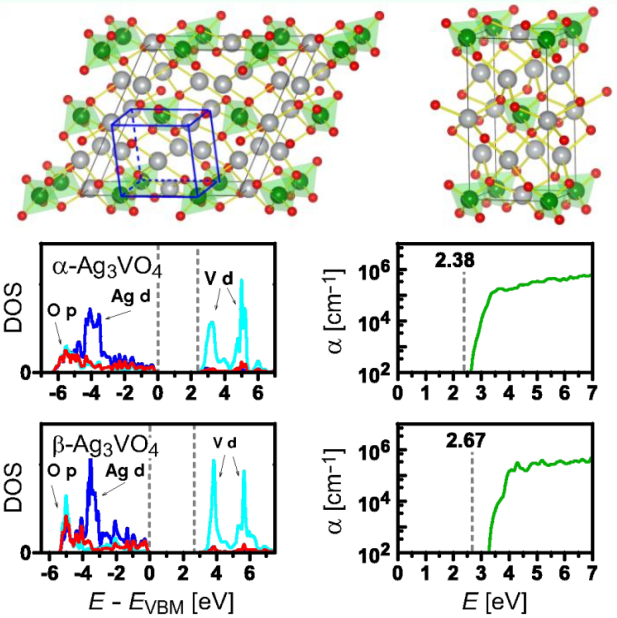
The Center for Inverse Design (CID) identified *silver vanadates* as a new class of *p*-type conductor, which are free from intrinsic hole-killing defects and have moderate transparency. β-Ag_3VO_4 was synthesized and measured at high temperature.

Significance and Impact

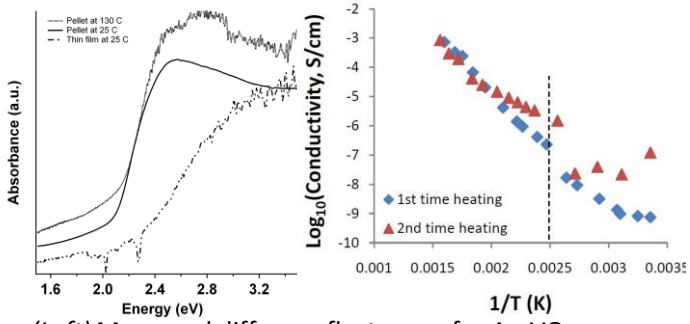
This work identifies a family of new *p*-type materials with potential to be good transparent contacts; key for improving the conductivity is the possibility for Cu substitution and doping.

Research Details

- *p*-type (hole-carrier) transparent conducting oxides are highly desired for photo-voltaics and display. However, to date, no *high-performance* materials are known.
- Using predictive theory, the CID identified Ag_3VO_4 as a promising *p*-type conducting oxide. In particular, *β*-Ag_3VO_4 appears attractive.
- Theory predicted an optical absorption edge of 2.6 eV for α-Ag_3VO_4 (with an indirect gap of 2.38 eV) and of 3.3 eV for *β*-Ag_3VO_4 (indirect bandgap at 2.67 eV).
- Ag_3VO_4 crystals, both the α- and *β*-polymorphs, were synthesized by a novel hydrothermal technique. The α-phase was predicted to be stable at room temperature and the *β*-phase at elevated temperature. Experimentally, we found the α-phase is stable below 365 K and the *β*-phase, although much more conductive, is only stable at elevated temperature.
- Attempts to stabilize the *β*-Ag_3VO_4 phase in thin-film form were unsuccessful by both sputtering and pulsed laser deposition.



(*Left*) Calculated density of states (DOS).
(*Right*) optical absorption profiles for Ag_3VO_4.



(Left) Measured diffuse reflectance of α-Ag_3VO_4.
(Right) Measured electrical conductivity of Ag_3VO_4 as a function of temperature.

V. Cloet, A. Raw, K.R. Poeppelmeier, G. Trimarchi, H. Peng, J. Im, A. Freeman, N. Perry, A. Zakutayev, P. Ndione, D. Ginley, J. Perkins, *Chem. Mater.* **24**(17), 3346–3354 (2012).

U.S. DEPARTMENT OF ENERGY | Office of Science | NREL NATIONAL RENEWABLE ENERGY LABORATORY | OSU Oregon State University | SLAC NATIONAL ACCELERATOR LABORATORY | Center for Inverse Design