Anti-Site Defects in p-Type Co_2ZnO_4: Better than Perfect

Scientific Achievement

The Center for Inverse Design (CID) demonstrates that intrinsic anti-site defects actually improve electrical properties of Doping Type II spinels, in agreement with prior CID prediction.

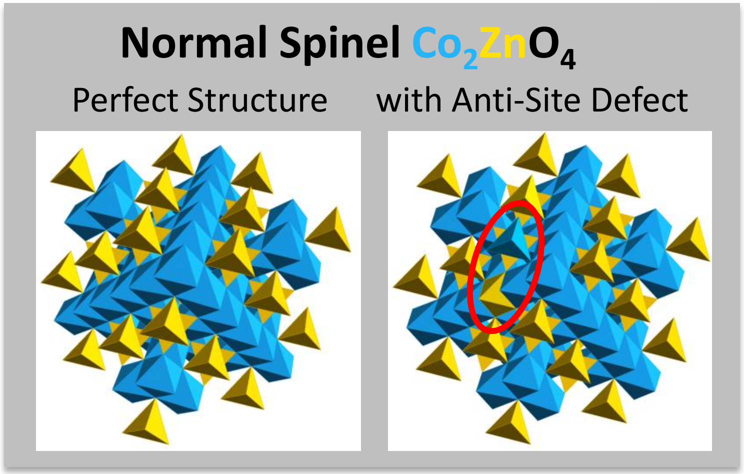
Significance and Impact

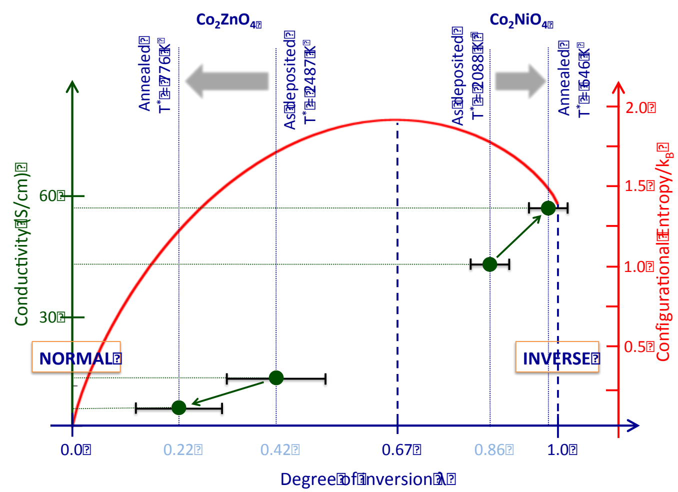
This work confirms a fundamental hole-generating process in Co_2ZnO_4, thereby enabling increased p-type conductivity via intentional non-equilibrium growth.

Research Details

- *p*-type (hole-carrier) transparent conducting oxides are highly desired for photovoltaics and displays. However, to date, no *high-performance* materials are known.
- The CID previously predicted via theory that anti-site defects should be a net hole producer for a special class of III-II *Normal* spinels typified by Co_2ZnO_4 and denoted Doping Type II.
- Resonant (variable beam energy) elastic X-ray diffraction (REXD) measurements done on as-deposited and annealed epitaxial Co_2ZnO_4 films confirm this prediction.
- For *Inverse* spinel Co_2NiO_4, spin-dependent electronic structure calculations predict Co_2NiO_4 to be a spin-polarized semi-metal.
- Consequentially, for Co_2NiO_4, decreasing defects through annealing is predicted to increase conductivity—just the opposite of the predicted effect for Doping Type II Co_2ZnO_4. This is also confirmed by REXD measurements.
- These new insights into the role of anti-site disorder underpin a new Design Principle whereby non-equilibrium growth is used to create beneficial disorder.

P. Ndione, Y. Shi, V. Stevanovic, A. Zakutayev, S. Lany, P. Parilla, J. Perkins, J. Berry, D. Ginley, M. Toney, *Advanced Functional Materials*, submitted March 2013.





(Top) Perfect and anti-site defect structures for normal spinel Co_2ZnO_4. (Bottom) Electrical conductivity in *Normal* spinel Co_2ZnO_4 and *Inverse* spinel Co_2NiO_4.

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