The Effect of Co, Ni, and Cr Impurities on the Properties of Iron Pyrite Single Crystals

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MOTIVATION

Iron Pyrite (FeS₂) is a promising photovoltaic material for multi-TW scale deployment.
- Strong light absorption (α > 10⁶ for hv > 1.4 eV)
- Suitable bandgap (E_g ~ 0.95 eV)
- Earth abundant, non-toxic

Progress has been limited, in part, by lack of understanding and control of doping. We conducted a detailed study of three transition metal’s (Co, Cr, Ni) effects on high purity, flux grown single crystals.

FLUX GROWTH

- Grown in Na₂S flux at 780°C
- High elemental purity (< 50ppm total impurities)
- Phase pure (XRD/Raman)
- Well characterized
- Pretty

OPTICAL

FTIR spectra – exploring sub-gap defect states

CONDUCTIVITY/HALL EFFECT

Doping Efficiencies

Co: Δn/Δ[Co] ~ s @ low [Co]
- Metallic behavior
Cr: Δn/Δ[Co] ~ 0.1 @ low [Cr]
Ni: Δn/Δ[Co] ~ 0

DFT (GGA+U)

Substitutional Co
- Defect state in CB
- .7 unpaired e (2+/3+)
- Some agreement between ε₂ & FTIR

Substitutional Cr
- Defect state in CB
- Cr²⁺
- ε₂ in poor agreement w/ FTIR

Substitutional Ni
- Defect state deep in gap
- Ni²⁺
- ε₂ reflects experiment

MAGNETIC

Oxidation states

Co: diamagnetic response (>2K)
- Co²⁺ low-spin (½2g½)

Cr: spin-only μeff/μB = 2.9 μB
- Cr³⁺ low-spin (½2g½)

Ni: spin-only μeff/μB = 3.07 μB
- Ni²⁺ (½2g½ ει½)

CONCLUSIONS

With a doping efficiency of ~50% at low concentrations and its high solubility, Co acts as a good n-type dopant. Which may be used to compensate the predominantly p-type thin films seen in literature. Cr does not contribute much to the number of free carriers, making it a poor candidate for doping. Except for causing low-temperature magnetism and some degradation in electron mobility, Ni by itself appears to be an inert impurity in iron pyrite.

REFERENCES


Fig. 1. FTIR spectra of undoped and transition metal doped pyrite samples. Arrows denote changes in absorption from the undoped case. Dashed segments are due to instrument artifact.