Center for Energy Efficient Electronics Science

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Thermoelectric Properties of Cadmium Oxide and Cadmium Zinc Oxide

Andrew Cook[1], Junqiao Wu[2], Bivas Saha[2], Scott Beaver[2]

[1]University of Maryland, Baltimore County

[2]University of California, Berkeley

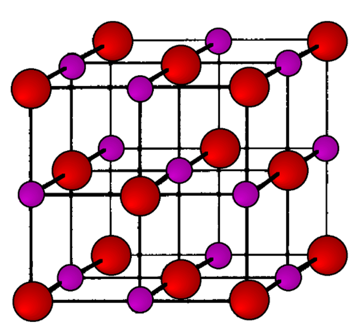
Abstract

The thermoelectric properties of the semiconducting oxide thin films cadmium oxide (CdO) and rocksalt-phase cadmium zinc oxide ($Cd_xZn_{1-x}O$) with x = 0.75 Cd concentration are characterized both computationally with the software Quantum Espresso and experimentally through the 3-Ω method. These methods determine the dispersion relation and specific heat, and lay the groundwork for measuring the thermal conductivity. Coupled with the high electron concentration, mobility, and infrared transmittance inherent in CdO films, this suggests viable heat transfer and dissipation properties appropriate for energy-efficient applications to transparent conductors often seen in photovoltaics.

Introduction

Motivation: Characterize the thermoelectric properties of CdO including:

- Thermal Conductivity
- Frequency at Brillouin Zone Origin
- Dielectric Constant
- Effective Charge
- Specific Heat
- Lattice Parameter
- Bulk Modulus



[1]

Rocksalt Crystal Structure

Background:

- CdO is a rocksalt-phase semiconducting oxide with a high electron density, high mobility, and band edge transmittance into the infrared range
- Applications to transparent conductors, such as photovoltaics

Computational Methods

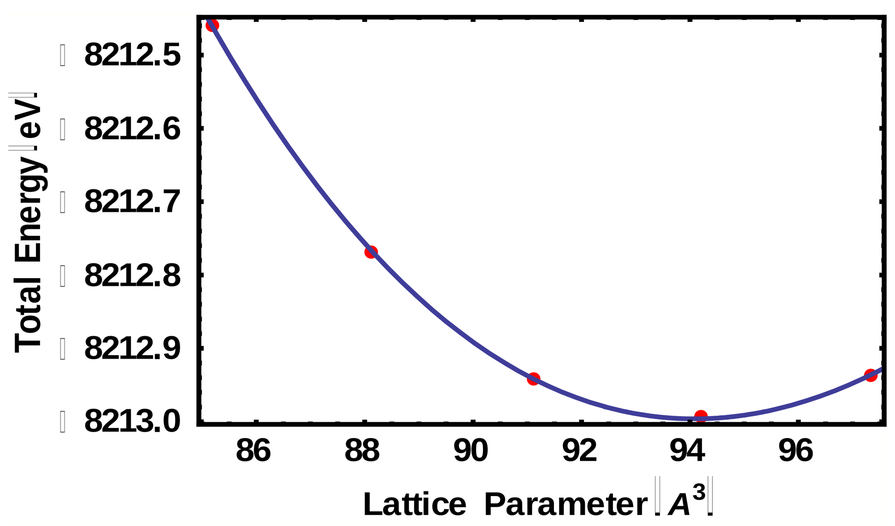
Quantum Espresso software used to calculate:

- Lattice Parameter
- Dispersion Relation
- Effective Charge
- Dielectric Constant

Resultant values fit with Einstein specific heat model to calculate heat capacity and thermal conductivity:

$$C_p = \frac{1}{N_q} \sum_{q\lambda=1}^{\infty} k_\beta \left(\frac{\hbar\omega_{q\lambda}}{k_\beta T}\right)^2 \frac{e^{\hbar\omega_{q\lambda}/k_\beta T}}{\left(e^{\hbar\omega_{q\lambda}/k_\beta T} - 1\right)^2}$$

[2]



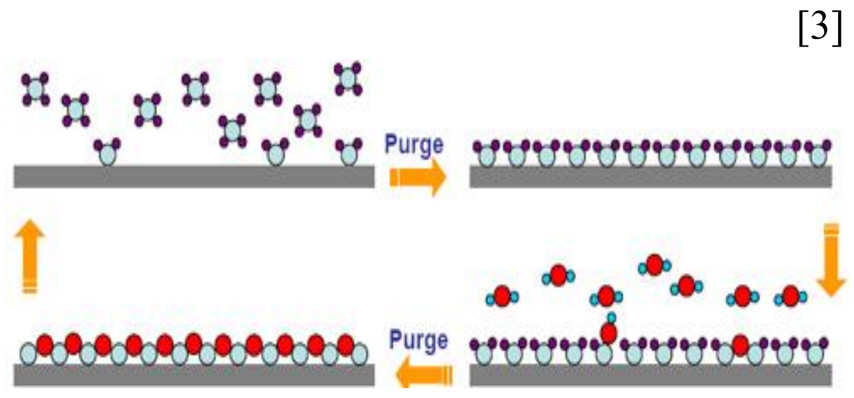
Lattice Parameter Optimization

Experimental Methods

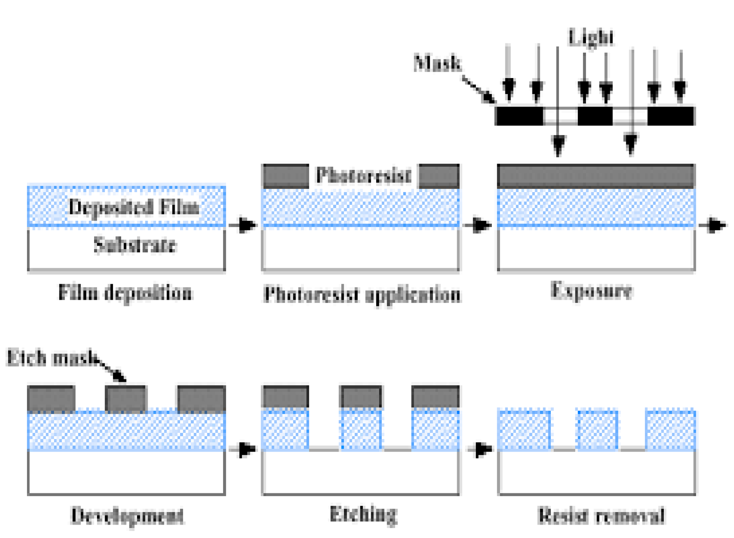
Atomic Layer Deposition:

ALD is a self-limiting reaction that alternates exposure of precursor gases to the substrate, facilitating chemical bonding in the creation of a metal-oxide thin film with precise thickness control

[3]



Spin-coating and Photolithography



[4]

3-Ω Method

- Measures thermal conductivity with metal heater-thermometer line
- Input frequency varies, affects third harmonic (V_3) and resistance of film
- $\Delta T = 2\,\frac{dT}{dR}\frac{R}{V}V_3$ plotted vs frequency yields linear fit
- Slope yields thermal conductivity

Results

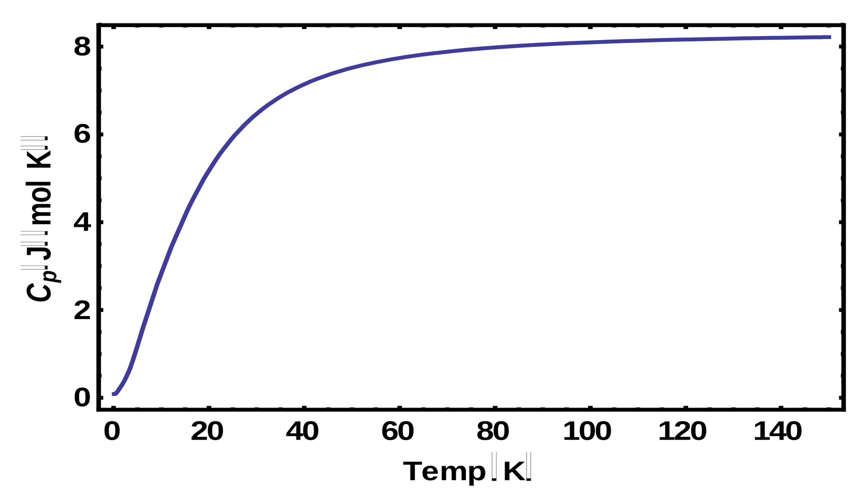


Fig 1. Specific heat vs. Temperature for CdO. Calculated with Quantum Espresso Phonon data and fit with Einstein's equation.

	Computational	Experimental
Lattice Parameter [Angstrom]	4.65	4.6942[5]
Bulk Modulus [Gpa]	151	150 [5]
Dielectric Constant	6.764	N/A
Effective Charge **(q*/e)**	2.40221	N/A
Gamma Frequency [cm^{-1}]	257.9, 431	262, 523[5]
Thermal Conductivity	In Progress	In Progress

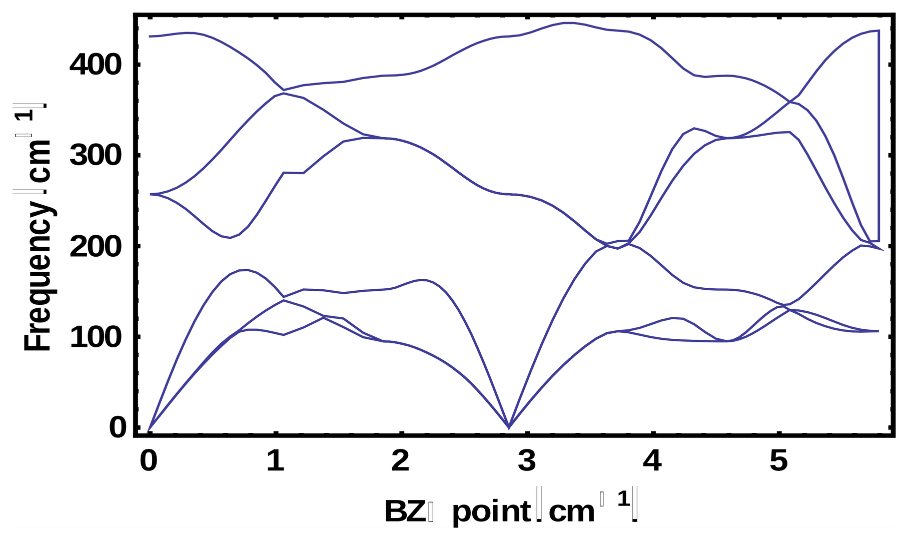


Fig 2. Dispersion relation of CdO, calculated using Quantum Espresso LDA. A dispersion relation can be thought of as every energy value that a phonon with a given momentum can occupy.

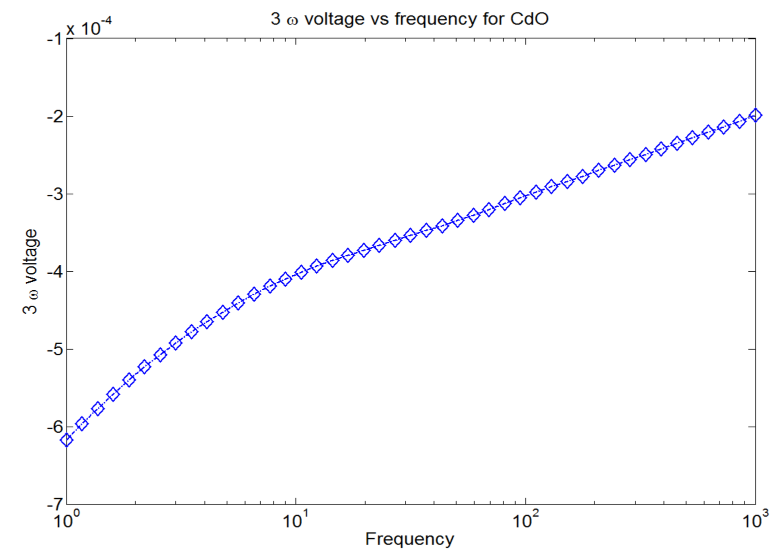


Fig 3. 3-Ω voltage plotted against the log of each input frequency. This voltage is caused by the third harmonic of the input current and can be used to calculate thermal conductivity.

Conclusions and Future Work

Conclusions:

- LDA calculation superior to GGA
- Two linear curves in 3-Ω measurement due to profiling of substrate, i.e. semiconducting oxide film too thin
- Specific heat curve seems unreasonably low, despite the frequencies agreeing with literature

Moving Forward:

- Calculate specific heat with more k-points for more accurate result
- Measure resistance at five temperatures from 290-310 K to determine dT/dR and thus, thermal conductivity
- Perform 3-Ω measurement for CdZnO
- Compare 0.75 Cd composition of CdZnO to CdO
- Determine which is superior for industry applications

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Contact Information

e: acook2@umbc.edu

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