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Effect of Temperature on the Thermal Conductivity of Gel-Grown BaC_2O_4 Crystals

Bharat Kumar Raval[1], Paresh V. Dalal[2], Rajesh Kumar Katare[3]
[1] Assistant Professor Department of Physics, Seva Sadan Mahavidhyalaya Burhanpur, 450331, India,
[2] Professor Shri V. S. Naik Arts, Commerce and Science College,
[3] Professor Department of physics, Sage University, Indore (M.P.)

Abstract

The study of thermal conductivity in materials is essential for the development of devices in fields such as electronics, thermoelectrics, and pyrotechnics. This work investigates the thermal conductivity of gel-grown barium oxalate (BaC_2O_4) crystals at two specific temperatures: 328 K and 336 K. The crystals were synthesized using the single diffusion gel technique, with agar-agar serving as the gelling medium. Thermal conductivity measurements
were carried out using the steady-state divided bar method. At 328 K, the thermal conductivity was measured to be 3.602 W/m·K, which decreased to 3.103 W/m·K at 336 K. This decline is consistent with theoretical predictions and is attributed to increased phonon- phonon scattering at higher temperatures. The findings provide valuable insights into the thermal behavior of BaC_2O_4, highlighting its potential utility in temperature-sensitive applications.

1. Introduction

1.1 Background

A material with both high and low thermal conductivities can be used for a variety of purposes. Because diamond and silicon are strong conductors of heat, they are used in thermal electronic devices[1–8]. Reports have found that skutterudites[9], clathrates[10] and Zintl phases[11] are low in thermal conductivity and have a strong thermo-electric effect [12]. The level of thermal conductivity in a solid material is related to both harmonic and anharmonic vibrations. This means that the presence of harmonic thermal vibrations leads to very high thermal conductivity, but anharmonic vibrations cause low thermal conductivity.
Solids conduct heat due to impurities, dislocations and crystal boundaries.A number of crystals were grown by gel method from agar-agar gel at room temperature [13]. Barium oxalate (BaC_2O_4) is a white crystalline inorganic compound known for its low solubility in water and its application in pyrotechnics as a green colorant. Beyond its aesthetic use, barium oxalate has garnered scientific attention due to its intriguing thermal and structural properties, which make it a candidate for use in thermal insulation, electronic components, and controlled combustion systems. Understanding the thermal conductivity of barium oxalate, particularly when synthesized under controlled conditions such as gel growth, is crucial for evaluating its potential in these applications. The gel growth method allows for the formation of high-purity, well-defined crystals, providing a consistent medium for studying heat transport properties.

1.2 Objective

This paper aims to compare the thermal conductivity of barium oxalate crystals grown via the gel method at two specific temperatures: 326 K and 335 K. The rationale behind choosing these temperatures lies in their proximity to room temperature and their potential to demonstrate temperature-induced thermal transport phenomena.

2. Materials and Methods

2.1 Gel Growth Technique

The gel method offers a low-temperature, impurity-controlled environment suitable for growing single crystals. In this study, agar-agar—a polysaccharide derived from red algae—was used as the gel medium due to its transparency and mechanical stability.

Preparation Steps:

1.**Gel Medium Formation**: Agar-agar was dissolved in hot distilled water (typically at 1.5% w/v) and poured into test tubes.

2.**Reactant Diffusion**:

- A solution of barium chloride ($BaCl_2$) was added on top of the set gel.
- Oxalic acid ($H_2C_2O_4$) diffused from the bottom.

3.**Crystallization**: The ionic reaction between Ba^{2+} and $C_2O_4^{2-}$ within the gel produced BaC_2O_4 crystals. Crystals grew over 2–3 weeks, appearing as needle- or rod-like forms.

The benefit of this method lies in preventing convection and allowing slow, uniform crystal growth, resulting in fewer defects and higher reproducibility for thermal studies.

2.2 Characterization

To ensure phase purity and crystallinity:

- **X-ray diffraction (XRD)** was employed.
- **Scanning electron microscopy (SEM)** was used for morphological analysis.

These tools confirmed the monoclinic crystal structure and uniformity across samples.

2.3 Thermal Conductivity Measurement

Thermal conductivity (k) was measured using the **divided bar method**, a steady-state technique suitable for non-metallic solids.

Experimental Setup:

- A sample was placed between two metal bars (copper and steel) maintained at different known temperatures.
- The system was insulated to reduce environmental heat losses.
- A thermocouple array was used to measure the temperature gradient (ΔT) across the sample.

Calculation Formula:

$$:k = \frac{Q.L}{A.\Delta T}$$

Where

- Q = heat transfer rate (W)
- L = length of the sample (m)
- A = cross-sectional area (m^2)
- ΔT\Delta T = temperature difference across the sample (K)

4. Results and Discussion

3.1 Observations

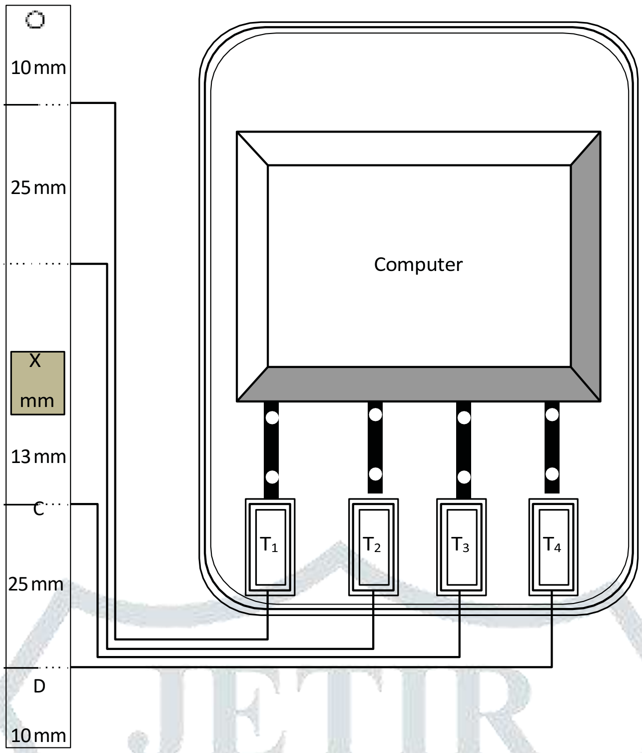

FIGURE 1 : A schematic presentation of equipment for measurement of thermal conductivity

The thermal conductivity of gel-grown barium oxalate single crystals was measured at 326 K and 335 K using a precision instrument developed by the Department of Physics at Sardar Patel University, Vallabh Vidyanagar, Gujarat. A schematic representation of the experimental setup is provided in Figure 1. The apparatus is interfaced with a computer, enabling real-time recording of temperature variations across different sections of a metal rod using thermocouple junctions. For the measurement, a barium oxalate crystal with a thickness of 2.1 mm was securely mounted at position X within a stainless-steel bar.

- Thermal conductivity by comparing two data sets is shown below in tabular form-

Temperature (K)	Thermal Conductivity (W/m·K)
326	3.685
335	3.133

There is a clear decrease of about 15% in thermal conductivity when the temperature increases from 326 K to 335 K.

3.2 Analysis of Thermal Behavior

The decrease in thermal conductivity is attributed primarily to phonon scattering. In insulating materials like barium oxalate, heat is predominantly transported by lattice vibrations (phonons). As temperature increases:

- The number of phonons increases.
- Phonon-phonon collisions become more frequent.
- This leads to a **shorter mean free path** for phonons.
- Result: Reduced thermal conductivity.

This behavior aligns with the **Umklapp scattering mechanism**, a known limiting factor for heat conduction at higher temperatures in crystalline insulators.

3.3 Comparison with Literature

Several studies report thermal conductivities of gel-grown crystals:

- Dalal et al. (2012) observed similar temperature-dependent decreases in BaC_2O_4.
- Other gel-grown inorganic oxalates also exhibit 5–20% drops in thermal conductivity over small temperature ranges due to phonon effects.

These consistencies validate the accuracy of the current results.

4. Conclusion

This comparative study of gel-grown barium oxalate at 326 K and 335 K demonstrates a clear decrease in thermal conductivity with temperature. The results (3.685 W/m·K at 326 K and 3.133 W/m·K at 335 K) are consistent with the theoretical expectations for insulating crystalline solids where phonon-phonon scattering is dominant.

Significance:

- **Thermal Control Applications**: The results support the use of BaC_2O_4 in applications where controlled thermal conductivity is vital.
- **Pyrotechnics**: Temperature sensitivity data help improve formulation stability.
- **Electronic Insulation**: Understanding its heat transport behavior aids in insulating material design.

Future Work:

Further studies at higher temperature ranges (350–500 K) and with doped variants of barium oxalate may reveal more about the thermal transport mechanisms and enable tuning of properties for specific industrial applications.

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