

# Determination of the Energy Bandgap of a Semiconductor Using Temperature-Dependent Resistance Measurements

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**In this experiment we measure the temperature-dependent resistance of a semiconductor sample and determine the band gap in the intrinsic regime. After carrying out the experiment we have for the band gap energy  $E_{g,T_2} = 1.129 \pm 0.003$  eV in a temperature range  $T_2 = [480.15, 773.15]$ K. We conclude that the experimentally obtained values do not align with the theoretical model and the literature value consequently does not lie within the uncertainty of our results. Therefore the experiment can be improved by conducting an extensive error analysis on the experiment setup and sample as well as finding more descriptive models and minimize simplifications to describe the behavior of the semiconductor sample.**

Microchips rely on semiconductor materials, which are essential in modern electronics. With of the sociotechnical influence of microchips nowadays comes also political as well as economical interest which emphasizes the importance of semiconductor materials.

Semiconductors are conductors whose charge carrier concentration and therefore its conductivity

$$\sigma = \sigma(T) \quad (1)$$

is temperature-dependent. At the atomic level, if  $N$  atoms are brought increasingly closer to each other and form a crystal, there is an increasing quantum mechanical coupling between the atoms. As  $N \rightarrow \infty$  the discrete energy levels of the isolated atoms form energy bands of allowed electronic states. This result can be obtained solving the following Schrödinger equation

$$\frac{\hbar^2}{2m} \nabla^2 u_{n\vec{k}}(\vec{r}) e^{i\vec{k}\vec{r}} + (E - V) u_{n\vec{k}}(\vec{r}) e^{i\vec{k}\vec{r}} \quad (2)$$

with spin degenerate energy states where  $u_{n\vec{k}}(\vec{r})$  is the Bloch function,  $E$  the total energy,  $V$  the periodic potential with the same period as the crystal lattice,  $m$  the free electron mass,  $\hbar$  the Planck constant  $\vec{k}$  the wave vector and  $n$  a band index. [1] [2] A consequence of solving Equation (2) using the *approximation for the quasi free electrons* is that solutions do not exist at all energies. Which explains the band gap

$$E_g = E_C - E_V \quad (3)$$

a range of energies where no electronic states exist, where  $E_C$  is the lowest conduction band energy and  $E_V$  the highest valence band energy.

The probability that a quantum state with energy  $E$  is occupied at a given temperature  $T$  is given by the Fermi-Dirac distribution

$$f(E) = \frac{1}{1 + e^{\left(\frac{E - E_F}{k_B T}\right)}} \quad (4)$$

where  $E_F$  is the Fermi energy,  $k_B$  the Boltzmann constant and  $T$  the temperature. Materials are classified via the position of the Fermi energy  $E_F$  at  $T = 0K$ .

- Metals:  $E_F$  lies within the conduction band, so electrons are free to move and contribute to electrical conduction. Conductivity is high ( $\sigma_{metal} \approx 10^5 \Omega^{-1} \text{cm}^{-1}$ ) and changes weakly with temperature.
- Insulators:  $E_F$  is in a large band gap ( $E_g \gtrsim 10$  eV). This makes them poor conductors ( $\sigma_{insulator} \in [10^{-14}, 10^{-3}] \Omega^{-1} \text{cm}^{-1}$ ).
- Semiconductors: The energy gap is smaller ( $E_g \lesssim 10$  eV) and an exponentially small number of thermally excited electrons populate the conduction band. Hence the electrical conductivity depends very sensitively on the temperature via Equation (4)

An ideal semiconductor, i.e. *intrinsic* semiconductor, has no lattice defects, impurities or dislocations.

A real semiconductor (*extrinsic*) contains at least a relative impurity atom concentration of  $10^{-10}$ . One can also voluntarily introduce impurities, i.e. dope the semiconductor, to fabricate *p-type* (achieved with acceptors) and *n-type* (achieved with donors) semiconductors, depending on the semiconductor material and the choice of atom to replace with in the crystal lattice. The consequence of doping is that it introduces different regimes of conduction. Namely an extrinsic and intrinsic conduction. In this experiment we study the intrinsic regime.

In the intrinsic regime conduction is dominated by the thermally excited charge carriers, i.e. for higher temperatures ( $k_B T \approx E_g$ ) which results in excitation of electrons from valence to conduction band. [3] The conduction is caused by electron-hole pairs and the charge carrier density is the following (under the assumption that  $E_C - E_F, E_F - E_V \gg k_B T$ )

$$n = p = n_i = \sqrt{N_C N_V} e^{\left(-\frac{E_g}{2k_B T}\right)} \propto T^{\frac{3}{2}} e^{\frac{-E_g}{2k_B T}} \quad (5)$$

where  $n$  is the electron density,  $p$  the hole density,  $n_i$  the intrinsic charge carrier density and  $N_C, N_V$  the effective density of states the conduction and valence band respectively. Lastly, the electrical conductivity is given by

$$\sigma \propto e^{\frac{-E_g}{2k_B T}} \quad (6)$$

[4]

## METHODS

The purpose of this experiment is to measure the electrical resistance of a silicon semiconductor sample as a function of temperature from room temperature to 873.15K. The resistance then is used to estimate the band gap  $E_g$  of the semiconductor performing a linear fit and extracting the slope using Equation (6), in order to compare the experimentally obtained values to literature values and therefore verify the theoretical model.

The experimental setup consists of a silicon sample, which has 4 aluminium strips evaporated on the surface to ensure good electrical contact to the wires on the bottom of the sample holder for a 4-point measurement, an oven and heat controller, as well as a vacuum pump. The sample is heated in a vacuum chamber in order to eliminate error sources or potential damage to the sample such as oxidation or thermal stress due to rapid heating or cooling. Furthermore a 4-point measurement is employed to measure the resistance of the sample, as it eliminates the influence of the contact resistances and therefore provides a more accurate measurement of the sample resistance.

Since the conductivity and hence the resistance is temperature-dependent as Equation (1) suggests, we first have to estimate a maximum current to avoid heating the sample since we do not have the temperature under control. Additionally, the temperature dependence of the resistance will lead to changes in the current and hence requires us to ensure that the estimated maximum current is not exceeded.

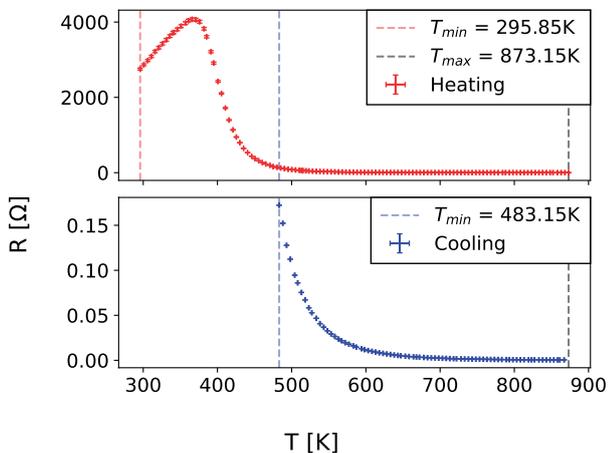
The measurement procedure consists of heating the sample from room temperature to 873.15K and cooling it down again to approximately the end of the intrinsic regime taking a datapoint every 5K.

## DATA ANALYSIS AND RESULTS

If not mentioned otherwise, the uncertainties of the values are calculated using Gaussian error propagation. (see Appendix A.1).  
data analysis

The estimated maximum current through the sample was estimated to be  $I_{max} = 0.55 \pm 0.05$  mA.

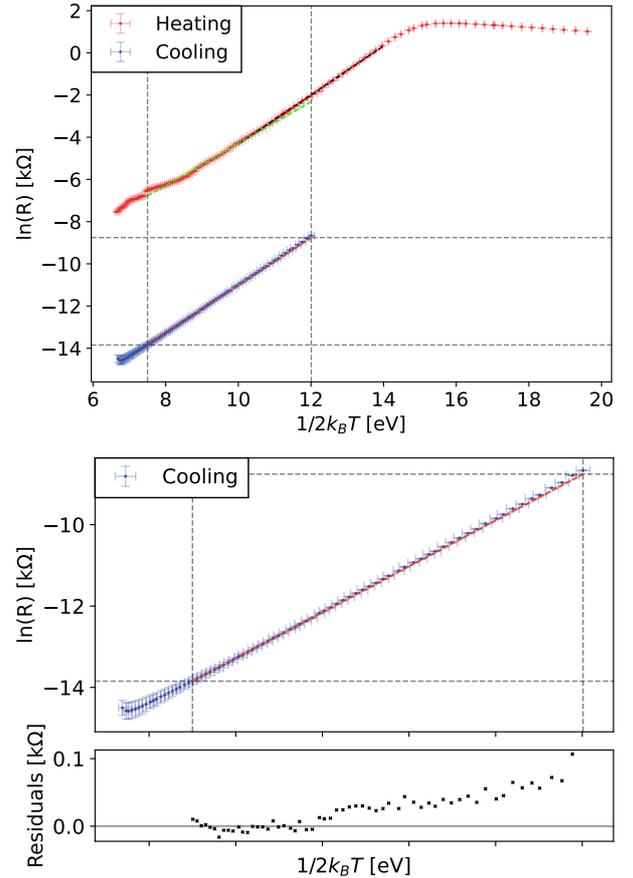
For the band gap determination the dimensions of the semiconductor were not relevant, therefore no further error analysis or measurements have been performed on it.



**Fig. 1** | Measured resistance of the semiconductor sample as a function of temperature, the upper graph for heating

the sample up to 873.15K and the lower for cooling the sample to approximately the end of the intrinsic regime  $\approx 483.15$ K. The datapoint at  $T_{max}$  is the same for both datasets and hence not considered in the lower one as it does not contribute to further analysis.

Since the electrical resistance is inversely proportional to the conductivity we can use the relation from Equation (6) to plot  $\ln(R)$  in dependence of  $1/2k_B T$ . We do this in order to be able to extract then from this relation through a linear fit the slope of the curve in the intrinsic regime which gives us the band gap  $E_g$ .



**Fig. 2** | The upper graph shows  $\ln(R)$  in dependence of  $1/k_B T$  for the heating and cooling process. To extract the band gap  $E_g$  a linear fit is performed in the intrinsic regime, the slope of the fit then is the value for  $E_g$ . To perform a linear fit, some values have been left out on purpose to ensure higher precision. The fits are indicated by the dotted lines. The black dotted line was chosen on a relatively linear behaving interval ( $T_1 := [410.65, 578.15]$ K) with as few fluctuations as possible. Hence all the values outside this range did not contribute to estimating the slope of the curve i.e. performing the linear fit. The same was done for the cooling process indicated by the red dotted line ( $T_2 := [480.15, 773.15]$ K), additionally the green dotted line then is the slope for the same interval the fit was performed on the dataset for the cooling process applied on the dataset for the heating process. The grey dotted lines emphasize the region of interest, which is also seen in the lower graph showing the dataset for the cooling process which is expected to have higher precision which shall be

used to compare with literature values.

Additionally for the linear fit on the cooling process the residuals have been plotted.

Using the the results of the fits, we can then compare the different calculated values for the bandgap  $E_g$  and compare to literature values.

**Table 1** | Estimated band gap  $E_{g,T_1}$  ( $T_1 = [410.65, 578.15]$ K) for the heating process as well as for the heating and the cooling process  $E_{g,T_2}$  ( $T_2 = [480.15, 773.15]$ K) using Equation (6). Furthermore the literature value for a silicon semiconductor at a temperature of 300K is listed even though it does not lie in any of our temperature ranges we used to perform the linear fit.

	$E_{g,T_1}$ (eV)	$E_{g,T_2}$ (eV)
Cooling	-	$1.129 \pm 0.003$
Heating	$1.164 \pm 0.005$	$0.99 \pm 0.02$

Literature Value for  $E_g$  [5]  
 $E_{g,T=300K} = 1.1242 \pm 0.0002\text{eV}$

## DISCUSSION OF RESULTS

As the values in Table 1 indicate, the estimated band gap for the cooling process is associated with a higher precision then for the heating process which was expected. Furthermore if one chooses the temperature range for the heating process in the most linear behaving region, the band gap for the heating process is closer to the band gap for the cooling process. It is expected since during cooling, the sample and its environment are more likely to reach thermal equilibrium at each step, which consequently leads to a more precise measurement of the resistance. In contrast, during heating, the oven introduces an active thermal input, which itself might fluctuate or be an uneven process, furthermore if the heating is rapid, the actual temperature of the sample might differ slightly from the recorded temperature. These are all systematic errors which were not considered in the error analysis.

Literature suggests a decline in the band gap with in-

creasing temperature, with the band gap at 300K being  $1.1242 \pm 0.0002\text{eV}$ . [5] Compared to our result of the cooling process  $E_{g,T_2}$ , the literature value does not lie within its uncertainty and is even larger than the value at 300K which does not correspond to the expected behaviour the theoretical model predicts since it should be smaller with increasing temperature.

The residuals of the fit are relatively small, indicating a good fit with minimal deviation from the model, which is expected in the intrinsic regime where the behavior of the semiconductor is dominated by intrinsic conduction. However as we move toward lower temperatures the residuals begin to increase, particularly at the right side of the plot. This could be explained due to the fact that extrinsic carriers start to dominate and therefore our model based on intrinsic behavior no longer holds, i.e. extrinsic conduction is not accounted for in our model since the material behaves differently which might not be described by our linear model anymore.

Additionally, since no error analysis on the semiconductor sample, regarding its doping or impurities, has been performed as well as above described systematic errors which were not accounted for the errors are expected to be much larger than calculated.

## CONCLUSION

In this experiment we determine the band gap of a semiconductor sample. The literature values and theoretical predictions do not lie within the uncertainty of our experimental results.

It is expected that this is a consequence of systematic errors included in the experiment setup, and under-descriptive models used to describe the behavior of the sample as well as only performing the measurement once which includes random error and hence falsifies the final results.

To improve the experiment, one should perform an extensive error analysis and assess the purity (or degree of doping) of the sample, the quality of the vacuum in the vacuum chamber and find a more descriptive model or use several models for different regimes acquired during the measurement process. Which will consequently lead to more accurate results and a better understanding of the behavior of the semiconductor sample.

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# A Appendix

## A.1 Calculation of Uncertainties Using Gaussian Error Propagation

For uncorrelated variables  $x_1, x_2, \dots, x_n$  with uncertainties  $\sigma_{x_1}, \sigma_{x_2}, \dots, \sigma_{x_n}$  and a function  $f(x_1, x_2, \dots, x_n)$ , the uncertainty of  $f$  is given by

$$\sigma_f = \sqrt{\sum_{i=1}^n \left(\frac{\partial f}{\partial x_i}\right)^2 \sigma_{x_i}^2} \quad (7)$$