Seeing Through Thin Films: A Model for Accurate Band-Edge Thermometry

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Background

Band edge thermometry provides a high precision, non-invasive way to measure the in-situ temperature of semiconductor thin films in vacuum. It works takes advantage of the relationship between bandgap and temperature, and is the basis for the k-space BandiT tool.

$$E_g(T) = E_g(0) - S_g k_b T$$

Linear relationship between bandgap and temperature

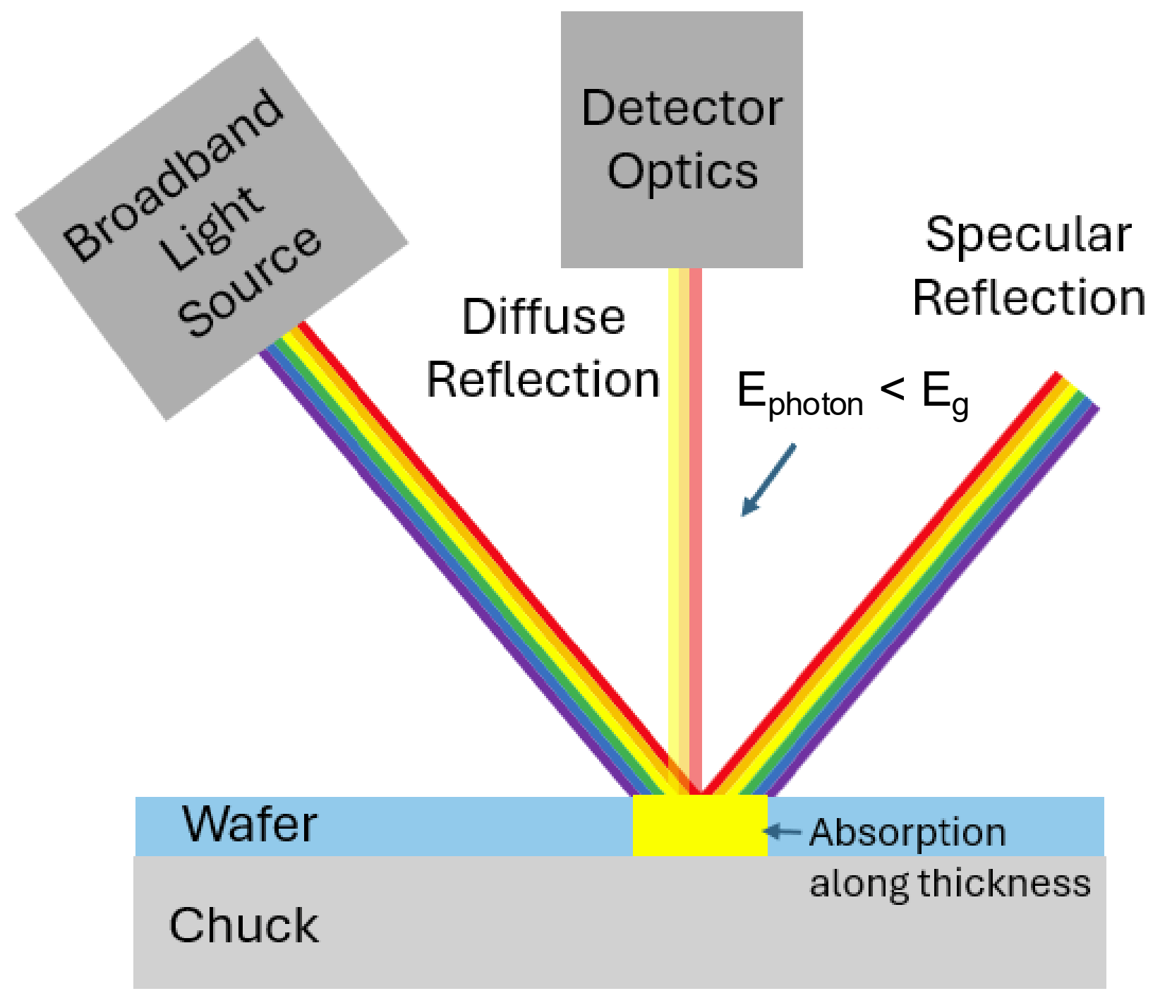
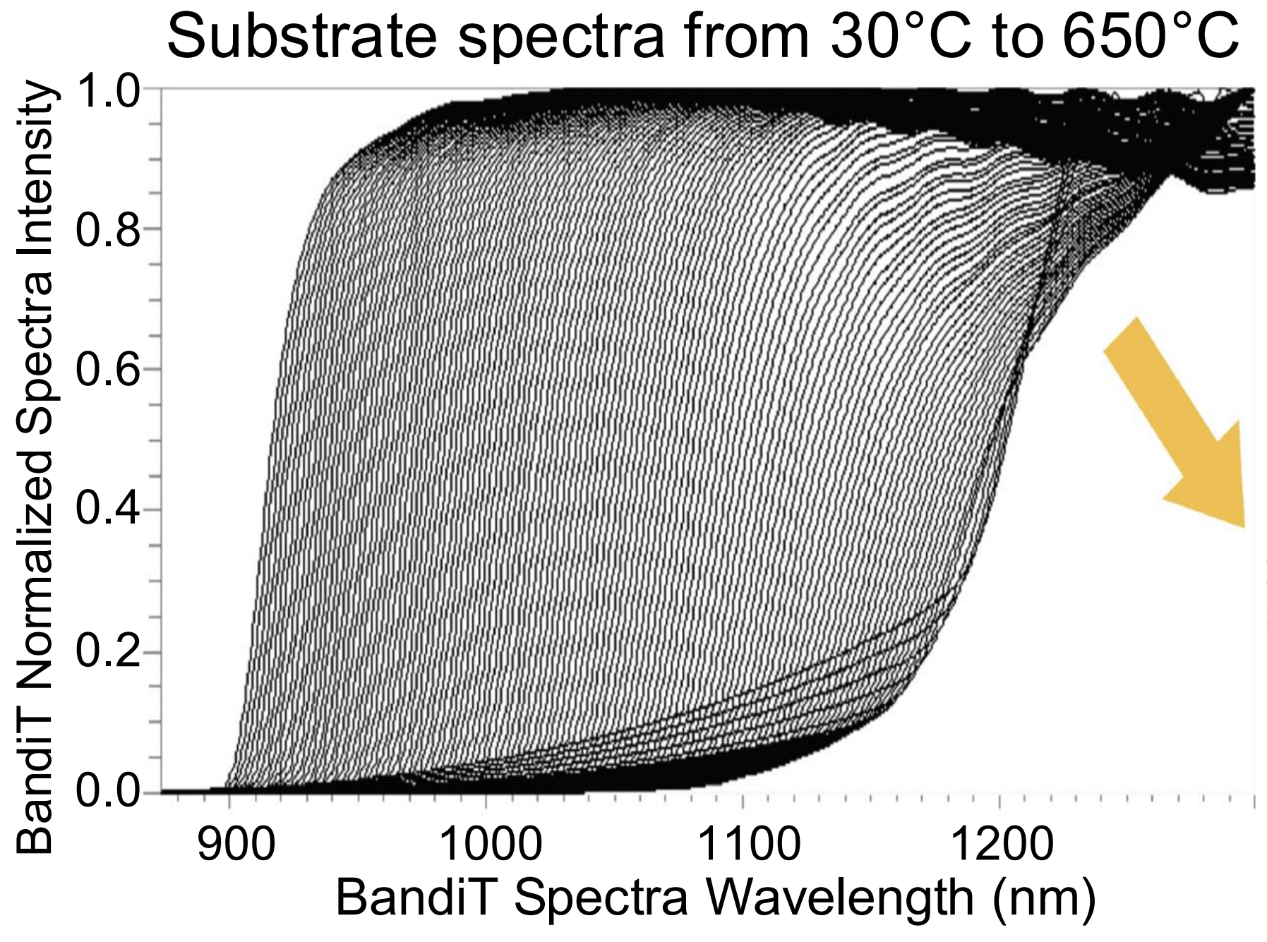


Figure 1: BandiT schematic[1]



Take spectra at many temperatures to produce a calibration curve

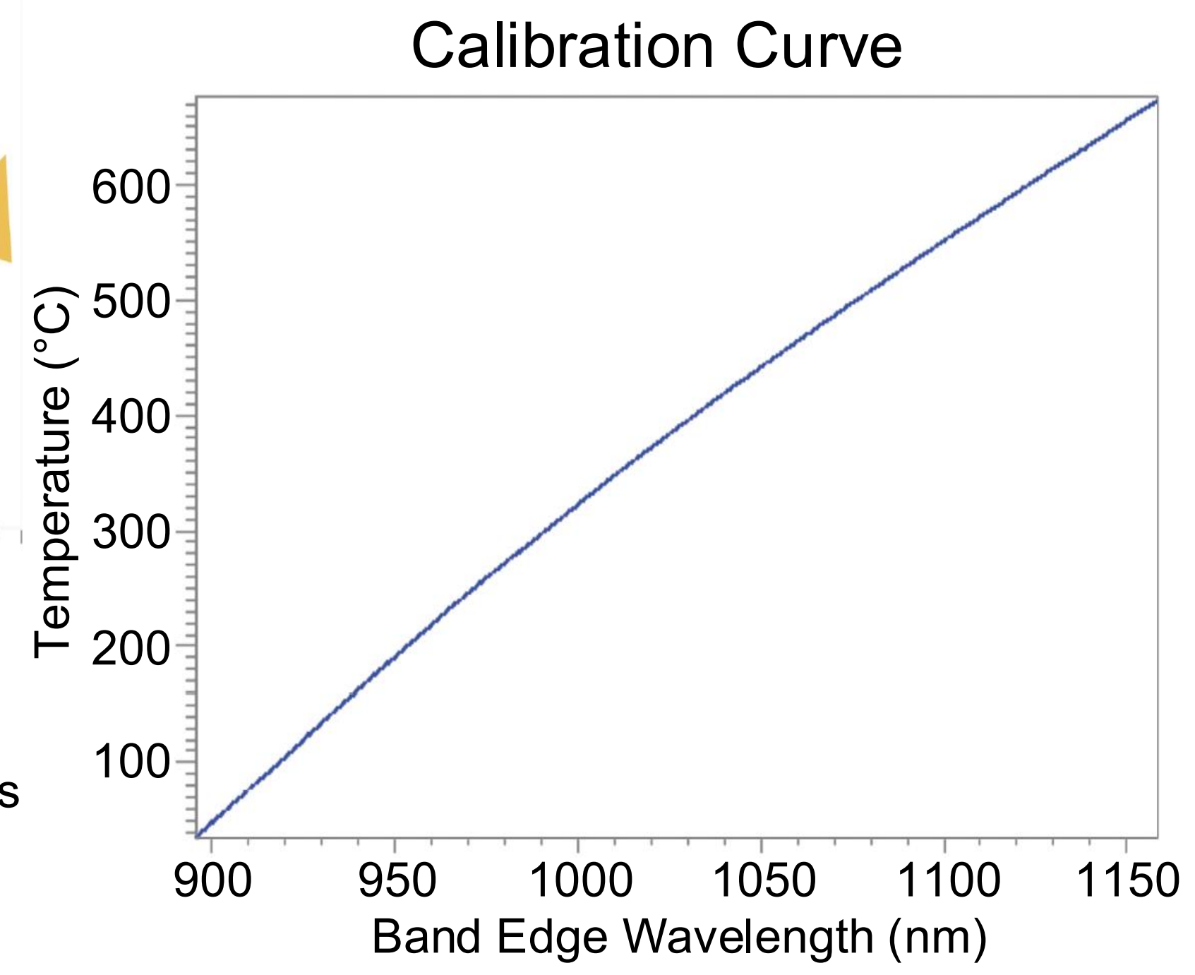


Figure 2: Generating a calibration curve of temperature vs band edge (R) by calculating band edge at many temperatures (L)

Objective

Problem: Calibration curves depend on substrate thickness, and take 9 hours to produce. A fast way to calibrate small deviations in substrate thickness is needed

Proposal: Develop a mathematical model to interpolate between thickness

Table 1: Specifications for a successful model.

Standard	Range	Confidence
Thickness	200-1000 µm	± 5 µm
Temperature	20-600 °C	± 10 °C
Material	Si p-type (B doped)	-
Goodness of fit	>0.9 (R^2)	-

Experimental Design

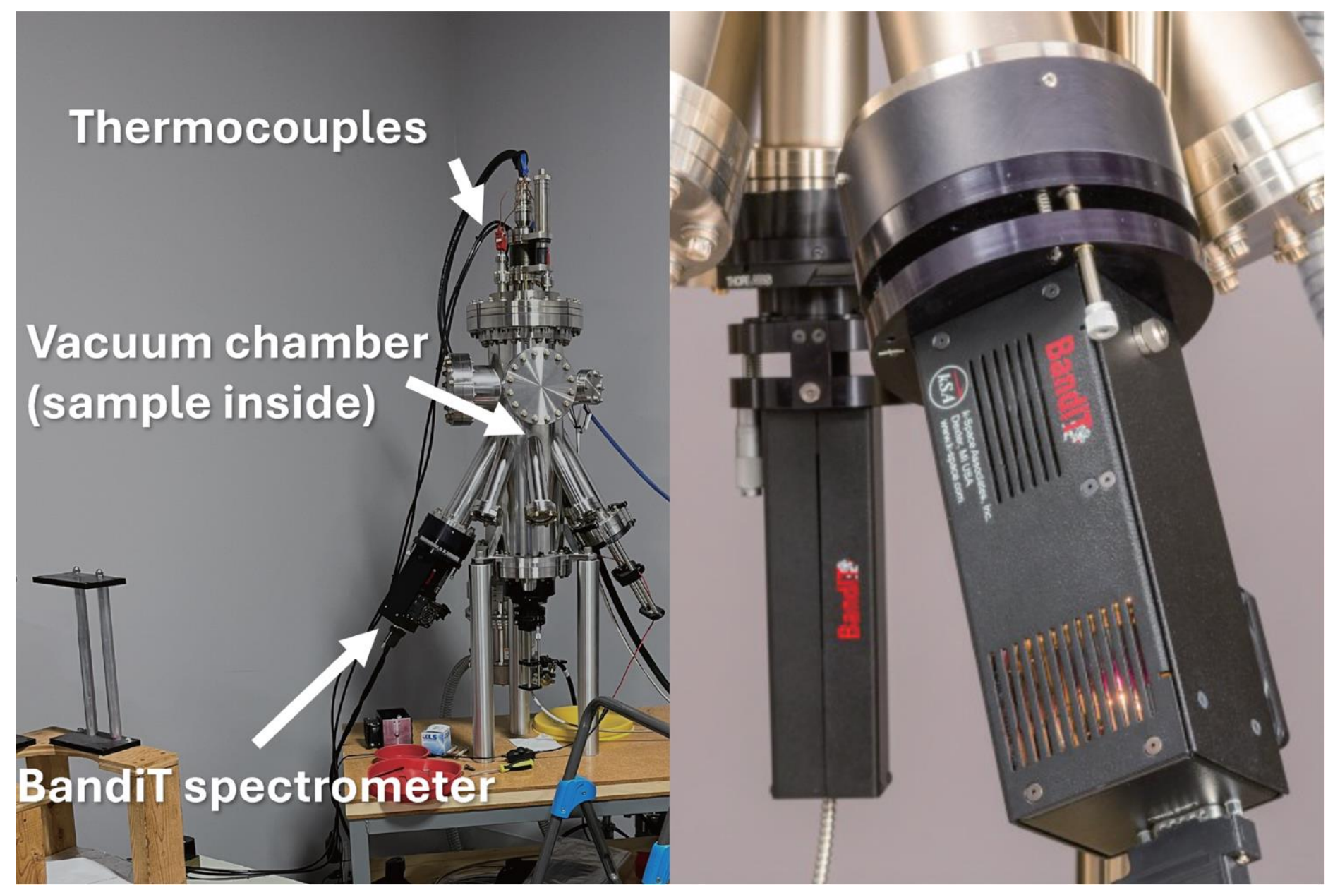


Figure 3: Data collection setup (L) and BandiT Spectrometer (R)

Each calibration curve for the model was created with this method:

- Measure sample properties
- Cut samples
- Prepare experimental setup
- Heat up sample to maximum temperature under vacuum
- Take band edge spectra with BandiT while cooling
- Process raw data[2]

Model Development

Model 1: Polynomial fitted coefficients

1. Take 3rd degree polynomial fit of raw data to produce the calibration curve relating observed Band Edge Wavelength to Temperature: $T(\lambda) = A + B\lambda + C\lambda^2 + D\lambda^3$
2. Assume that the constants A, B, C, and D are quadratically dependent with thickness d
3. The temperature curve is now: $T(\lambda,d) = A(d) + B(d)\lambda + C(d)\lambda^2 + D(d)\lambda^3$, where $A(d) = A_1 + A_2d + A_3d^2$, with B, C, and D being the same
4. Perform a least squares regression fit on $T(\lambda,d)$ using existing calibration curves

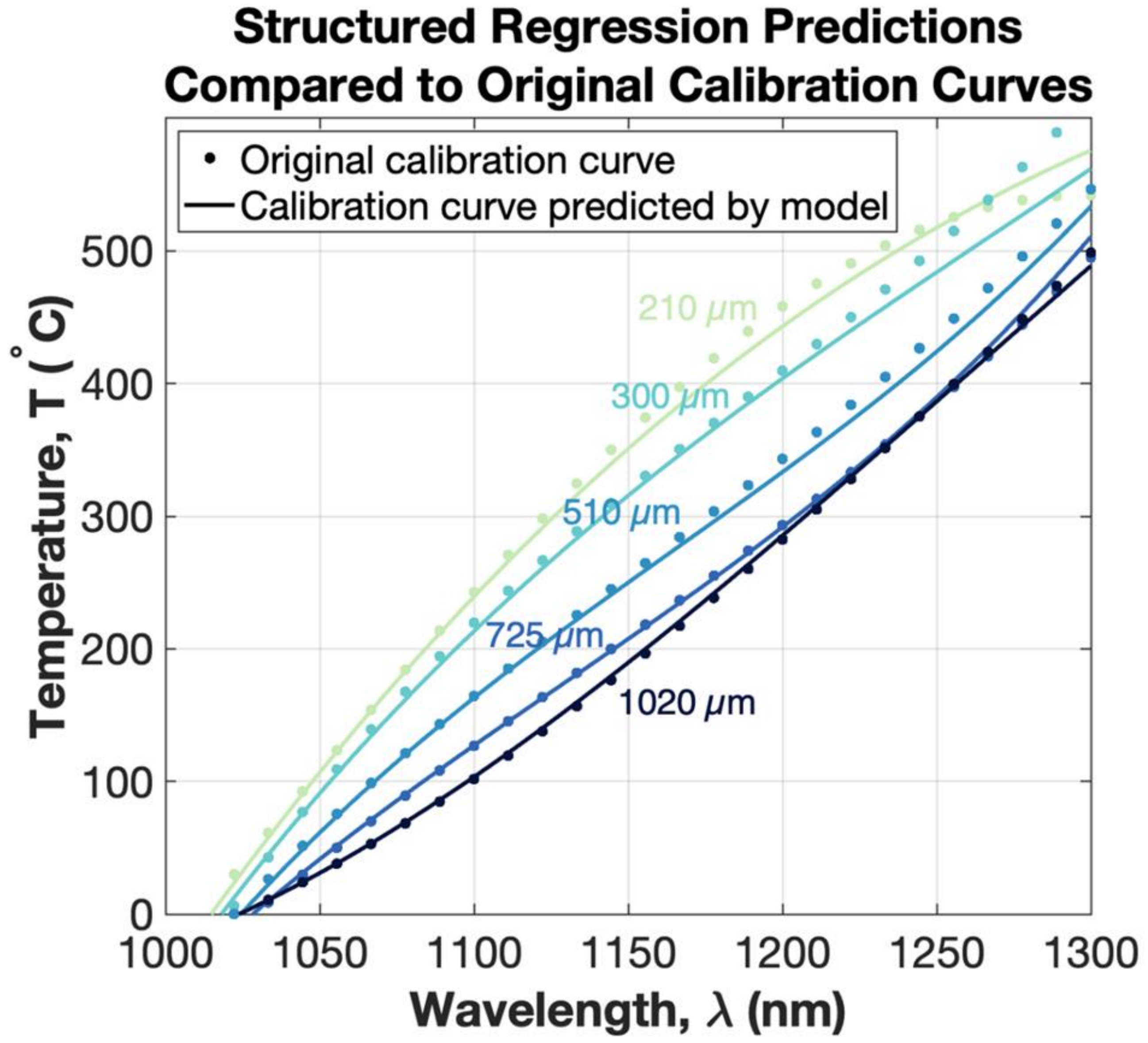


Figure 4: Polynomial fitted coefficient model prediction vs. original calibration curves

Model Development (Continued)

Model 2: Linear + gaussian raw data fit

1. Use raw low and high temperature data to estimate a linear fit
2. Add a gaussian fit for the residuals of the "hump" region
3. Combine both fits into one function

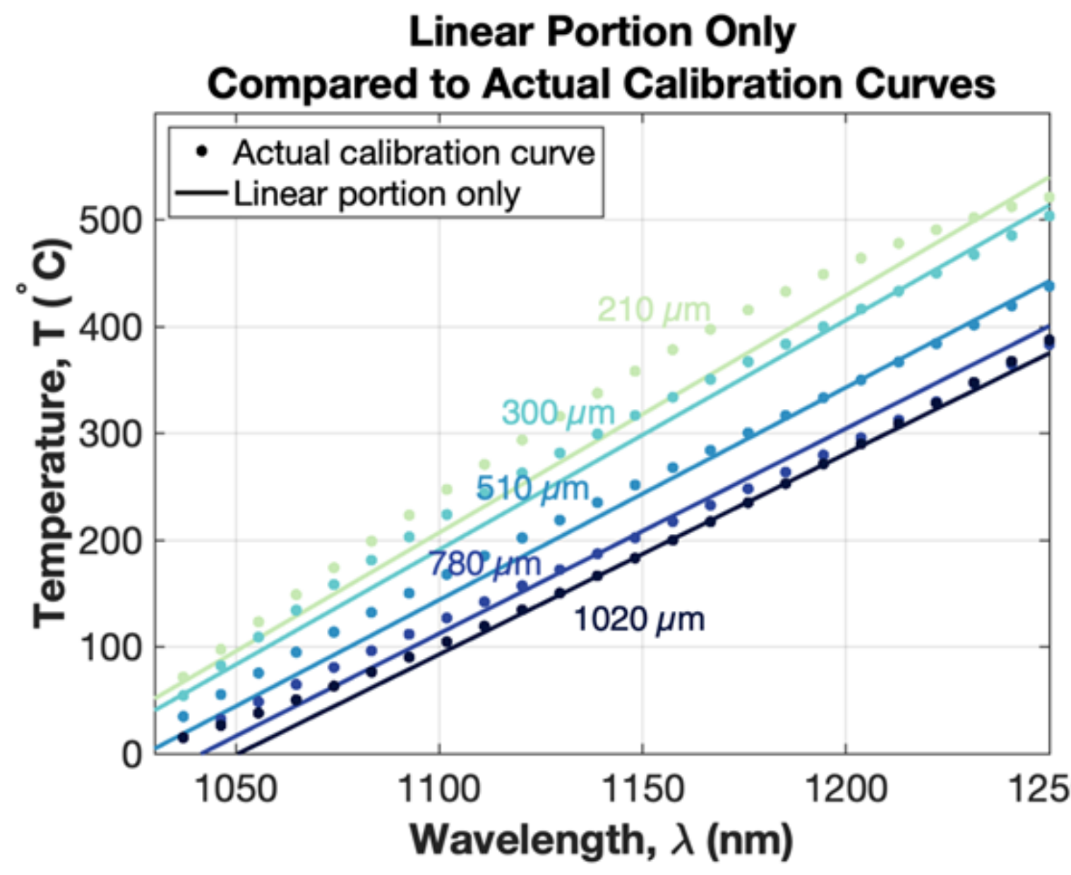


Figure 5: Linear fit vs. calibration curves

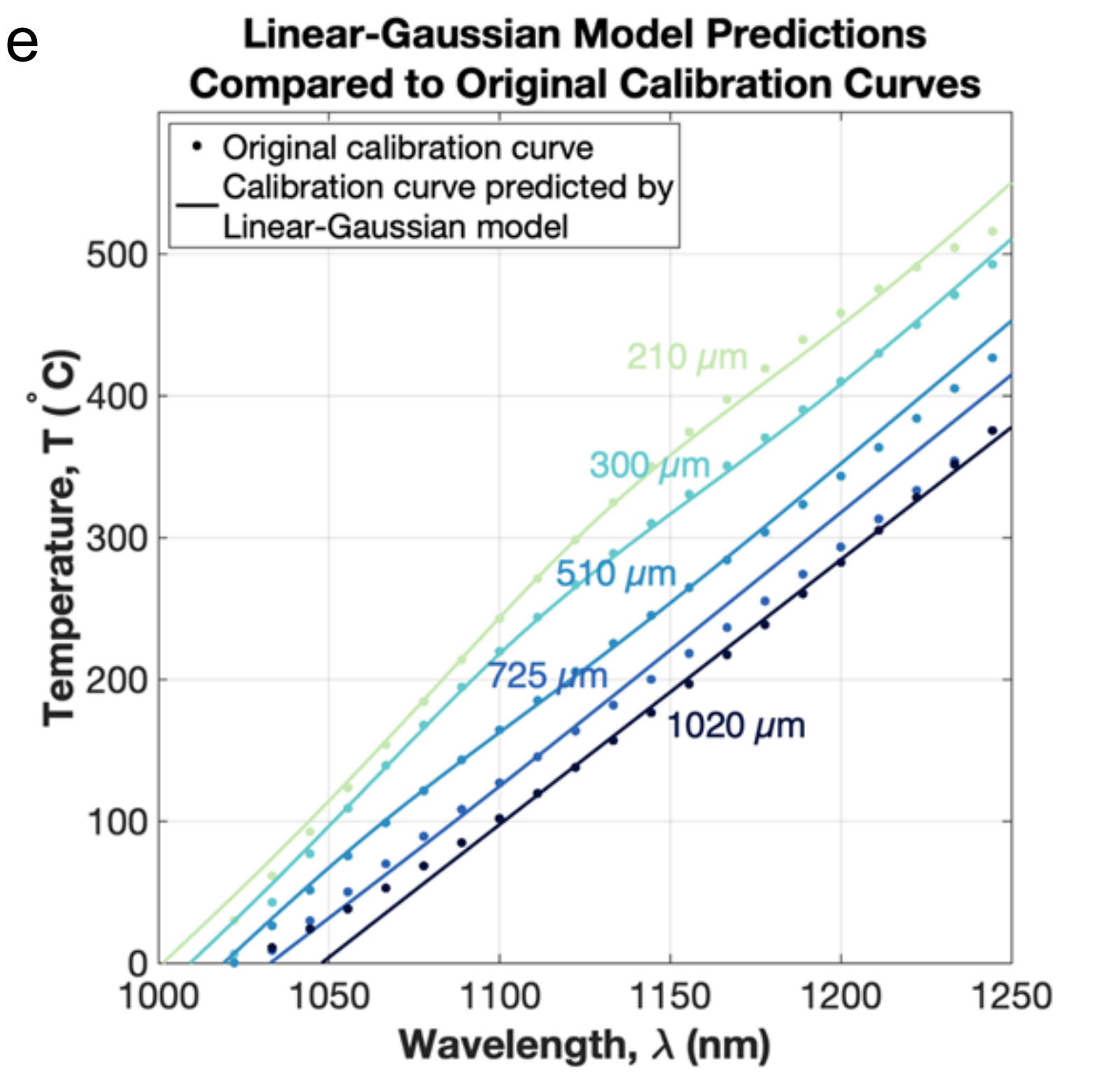


Figure 6: Linear-Gaussian fit vs. calibration curves

Conclusions

Table 2: Model performance

Model	R^2	RMSE (°C)
Model 1	0.993	14.26
Model 2	0.986	13.97

Both models give similar, highly predictive results. R^2 requirements are met, but both models fall short of error specifications.

Impact and Future Work

- **Impact**
  - Saves large amount of time testing to generate new Si calibration curves
  - Provides intuition on how substrate thickness relates to shifts in curves
  - Save resources while providing high quality semiconductor growths
- **Future Work**
  - *Collect more data:* too small of a sample size for a truly accurate model
  - *Dopant concentration as a parameter:* dopant changes chemistry, thus shifting the calibration curves, but it was a control variable in our model
  - *Generate new models for materials beyond Si:* such as GaAs and InP

Acknowledgements

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References: [1] Barlett et. al, "THIN FILM TEMPERATURE MEASUREMENT USING OPTICAL ABSORPTION EDGE WAVELENGTH," K-Space Patent, 2014. [Online]. Available: https://patentimages.storage.googleapis.com/8d/d5/3f/e81e59f00ad9b8/US8786841.pdf
[2] Barlett et. al, "BLACKBODY FITTING FOR TEMPERATURE DETERMINATION" K-SpacePatent,2015.[Online]. Available: https://patentimages.storage.googleapis.com/35/85/24/6d7f31f281d6db/US8282273.pdf

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