High-Throughput Measurement of Deep Eutectic Solvent Melting Points using IR Bolometry

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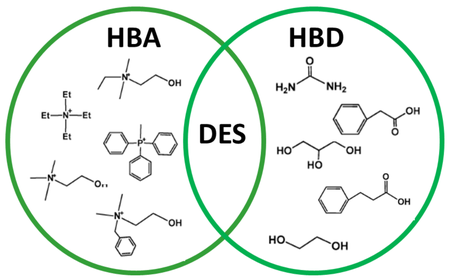
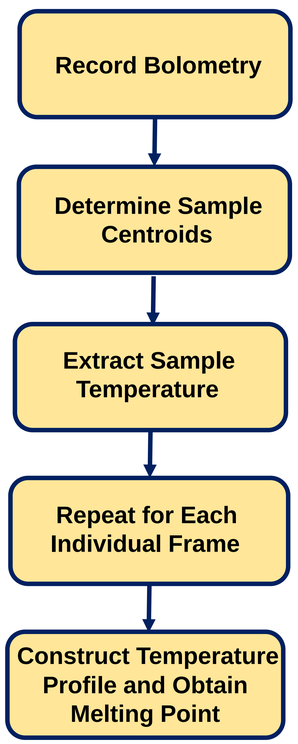
Background and Motivation

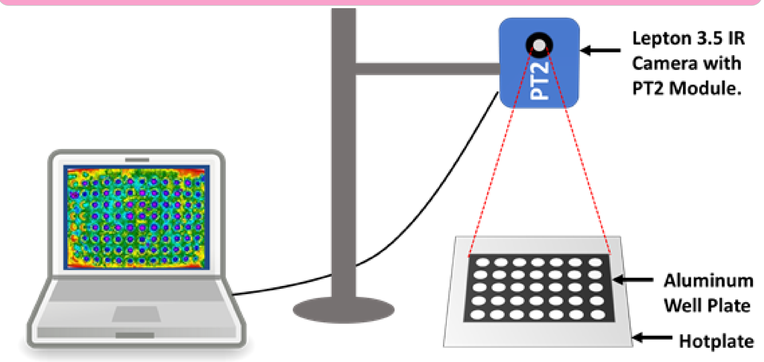
Deep eutectic solvents (DES) are novel solvents formed between organic hydrogen bond acceptors and donors. DES can be formed at low-cost for several important applications, such as chemical synthesis, extractions, electrochemistry, and even drug delivery. However, the design space for DES is enormous and high-throughput measurement of melting points is required to rapidly identify DES with melting points that are feasible for their intended application.



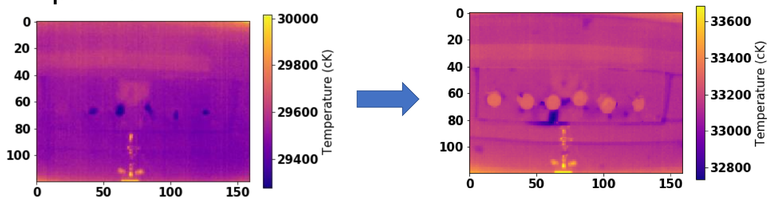
Workflow



Bolometry Setup

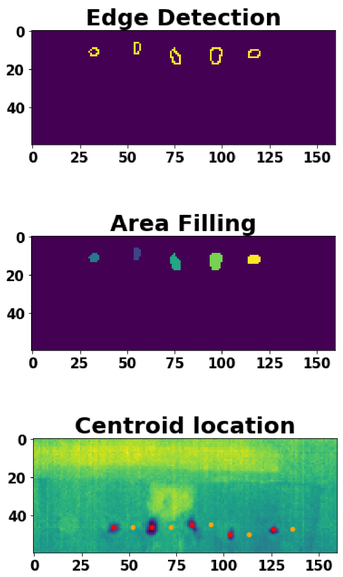


- Sample temperature is monitored by an IR camera.
- Melting points are detectable from a sudden increase in sample temperature due to an increased thermal conductivity in the liquid phase.

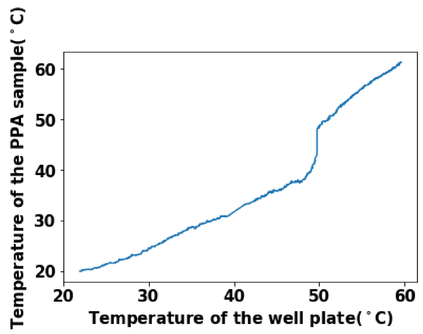


Solid Sample **Melted Sample**

Temperature Profile via Edge Detection

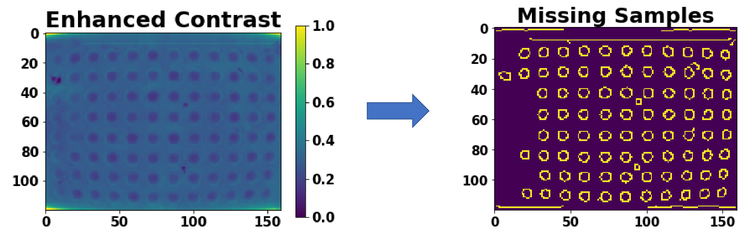


- The temperature profile of the samples and plate is determined by detecting the edges, filling and labeling them, and monitoring the temperature at their centroids.

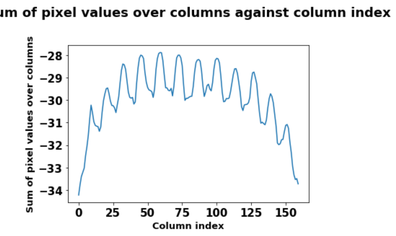


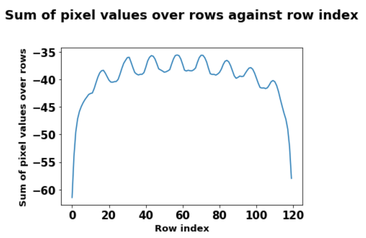
Alternative Method for Low-Contrast Samples

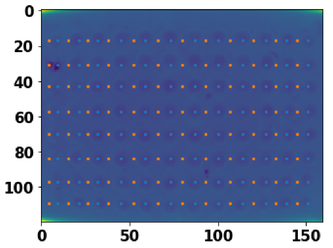
- In some situations, the contrast between the image and sample may be too low for edge detection, even with contrast enhancement.



- Alternatively, centroid locations for each sample can be found by summing pixel values over individual rows and columns of the sample holder (well plate).







- Using this alternative method, centroids were located for each sample in a 96 well microplate.

Conclusions and Future Work

Using IR Bolometry, melting points can be determined for multiple samples at once in a matter of minutes, as opposed to standard techniques which may take up to an hour for a single sample. Once sufficient data is collected, future work may include the development of a machine learning model to predict the melting points of DES based on their composition.

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