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***Abstract*— The Infrared Spectrometer is a device mainly used by chemists to allow the searching of a single molecule throughout a solution. Each bond absorbs a set frequency of infrared light and one could use that knowledge to figure out when there is a certain bond in your solution. It also allows the bond selected to 'light' up in the output. The main drawback of a standard infrared spectrometer is that it only is allowed to look at a single pixel and average it all together where the one I am creating is going to be two dimensional and selective time averaging. The research I have done here is to gain a better understanding of the technology itself, but to also see what worked and what didn't work for many others and try to implement their successes where they fit.**

I. INTRODUCTION

The senior project that I have chosen is to create a two dimensional, selected time averaging infrared spectrometer. A standard infrared spectrometer works by utilizing an infrared laser and an infrared camera. The laser is directed via mirrors towards a capture point where the sample to be tested is. The ray of infrared light is then directed to the capture point of the spectrometer's camera. This process is only done for a single pixel. The infrared spectrometer measures how molecules react to the infrared light. Once hit by the light, the molecule will vibrate in a certain way, which is decided by the electronegativity of the molecule itself, as well as the actual wave length of the infrared beam. When the molecule is vibrating, it absorbs more the infrared beam than it would if it was not vibrating. The infrared spectrometer measures the amount of infrared light that is absorbed because a certain molecule will absorb the peak amount of infrared light at the same wave length each time. The practicality of this is to find if there is a certain molecule in a solution or to watch a reaction take place.

A standard infrared spectrometer only measures this absorption over a single pixel, while the one I am helping create is doing all of this for a resolution of 320 x 240 pixels, which equates to 76,800 individual pixels. Another feature of the infrared spectrometer used in my senior project is that it will have selected time averaging. Selected time averaging is using the infrared spectrometer to take multiple images at a given frequency, then averaging the frames captured into a single image. This is done to reduce noise, or unwanted background, as much as possible which is necessary because, currently, there is no enclosure at all. The enclosure is a physical barrier to the system that is needed to limit the amount of water vapor and carbon dioxide. An infrared spectrometer achieves the best results when there is no water vapor or carbon dioxide, because these add noise and interfere with the data. In addition to averaging all of the frames together, we have the ability to select any connected pixels and have them averaged together. This advancement is an incredibly important aspect to the final product because it allows for the analysis of multiple samples at the same time. When observing a sample reaction, one could have a boundary set up so there are several reactions or solutions in a single frame, cutting down the time it takes to gather data on samples by up to six times.

Once the whole system is up and running, the chemistry department has research that they want to complete utilizing this piece of equipment. They want to test different solutions to see which one will have the greatest potential to become the next compound for batteries. This type of experiment almost requires a 2D Infrared Spectrometer because it allows them to compare the different solutions side by side in the same test.

II. ROTATING FRAMES

Since the creation of two dimensional infrared spectrometers, the chemistry community has worked hard to quicken its process. Currently, depending on the laser and camera used, it takes about 10 minutes to completely cycle through the available wavelengths on the laser. This may seem like a short amount of time but the people who use this every day for research do so up to a hundred times a day. Therefore, the possibility of reducing this time to just a minute or two not only increases

the productivity of the individual person, but also the advancement of the research itself. This cycle time decrease is attributed to rotating frames. Although the setup is many times more complicated than two dimensional infrared spectrometers, some argue that it is worth the extra time to set up and money. Another potential problem is that when using rotating frames, the actual data is less precise, which the user would have to take into account. Usually, the impreciseness only shows up when looking at molecules that are not absorbing a significant amount of light. Recently, however, there have been several discoveries that have made rotating frames almost as accurate as not using them. Such research is being done by Karthick Kumar, which he explains in his Journal, Comparisons of 2D IR measured spectral diffusion in rotating frames using pulse shaping and in the stationary frame using the standard method:

"We have implemented a pulse-shaping based 2D IR vibrational echo experiment in a pump-probe geometry. Data were taken using … a stationary, a partially rotating, and a fully rotating acquisition frame. The spectra themselves, resulting from these data as well as the data previously acquired using a standard delay line setup, were found to be identical within the noise. Furthermore, the spectral diffusion information derived from them, in the form of a CLS analysis, was shown to be the same regardless of origin. The speed of data acquisition and the quality of the CLS derived from the pulse-shaping setup were both found to be superior to those derived from the standard setup. "[1]

In the above selection, Kumar talks on his results of his experiments, showing that he has developed a rotating frames method where it is as accurate and quicker than normal two dimensional infrared spectrometers.

III. Sum-Frequency Generation

Although there are no purchasable versions of a two dimensional infrared spectrometer, there are many that have been built, just as I am building my own. These two dimensional infrared spectrometers are being used for all sorts of different yet important research. Wei Xiong and colleagues implemented a version of two dimensional infrared spectrometer using a technique called heterodyne detected HD two dimensional sum-frequency generation. [2] This sum-frequency generation allows the user to quickly go through each individual frequency and bring that data together to allow for extremely high level view of what sample you are looking at.

IV. Purpose of Research report

The research report provides several important pieces of information that are crucial to the success of this project. Although it was very difficult to find papers that correlated with my specific project and that were not so advanced that I could not understand them, the several I did find have become extremely useful. One of these in particular, explained several things that when setting up a 2D Infrared Spectrometer, one could easily do wrong.

V. Functionality

When building an instrument such as this for a group of people who do not have the required technical skills to make changes as they see fit, it is important to have set functions that they can use for all of their work.

A. Calibrate mode

When the system is put into calibrate mode by the user or automatically, it will run a thorough scan to get a good idea of the ambient values so when run in experiment mode it will produce a set of background images for the specified IR frequencies of the laser light. Optionally, a specified number of frames will be used to produce background images with lower noise level.

B. Experiment configuration mode

In the experiment configuration mode, the user has to input the frequencies for the laser beam along with the time to average images for each frequency, and the overall time of the recording. This set of data may be followed by more sets of the same structure. Multiple configurations can be stored under different file names

C. Experiment mode

The system will power on the laser, if not already on, and then will perform the IR laser control and IR image recording according to the data stored in the experiment configuration file.

D. *Result computation mode*

The prerecorded results of the experiment are compared with the background/calibration image for the user-selected area(s) of the image. The data file for the visualization of the results are prepared and stored in the file. Then a program to visualize the results is run. Programs such as Libre Office Spreadsheet, GnuPlot, and Octave (GNU Matlab equivalent) are considered for the final visualization.

VI. SYSTEM LEVEL DESIGN

The system level design document is used to describe the inputs and outputs of the system as a whole.

A. *Inputs:*

- Request to calibrate, it is necessary to calibrate the system before use when external environment has changed activated by user.
- Request to immediately power up or power down the laser.
- Power to the camera, laser and computer.
- Request to start the experiment according to the specification stored in a configuration file, this has many inputs such as range of laser frequencies, time to be averaged, and the overall time of recording.
- The configuration file for the experiment.
- Request to process the experiment results for the selected area or areas of the sample.

B. *Outputs:*

- Archived background image/calibration data.
- Archived partially-processed 2D images from the spectrometer.
- Final processed images.

VII. WORK COMPLETED TO DATE

The work that I have been mostly completing for the first portion of this project is learning and teaching. Right away, I had to take a crash course on not only Infrared Spectrometers but also chemistry as a whole, to really get a firm grasp on what it is that I am dealing with. Once I learned what the Infrared Spectrometer does, I was able to start teaching the two chemistry students how to do work the program that was created. This involves constantly being on call for them, coming into the lab whenever they require my assistance. While doing this over the semester, I have also updated to layout and implemented several new functions to the GUI that the students use daily.

VIII. DELIVERABLES

For ECE 499, there are several deliverables that I came up with. Since I am the only member of my group, I do all of the labor myself. As talked about in presentation, this type of project works best with a dynamic ‘to do’ list, meaning there is no hard schedule for when things should be done. In terms of the parts that I am working with, there is the computer, infrared laser, infrared camera, motors and the actuator.

IX. CONCLUSION

While we are still in the process of constructing the two dimensional infrared spectrometer here at Bradley, I can use this research I found to improve it past what we initially thought it would be. Once the infrared spectrometer is finished here at Bradley, the chemistry department has plans to study how batteries charge and discharge over time. This will be done by applying charge to some of the molecules in the sample while having another section already charged. Through the replay feature of the code I am writing, one will be able to watch what happened with the ability to pause, and go frame by frame. The resulting new information this data will yield could lead us to batteries that hold more charge and could charge quicker than current commercial ones.

X. References

[1] S. K. Karthick Kumar, A. Tamimi, and M. D. Fayer, "Comparisons of 2D IR measured spectral diffusion in rotating frames using pulse shaping and in the stationary frame using the standard method," Journal of Chemical Physics, vol. 137, no. 18, p. 184201, Nov. 2012.

[2] Wei Xiong, "Adding a dimension to the infrared spectra of interfaces using heterodyne detected 2D sum-frequency generation (HD 2D SFG) spectroscopy," Proceedings of the National Academy of Sciences of the United States of America, vol. 108, no. 52, pp. 20902–20907, Dec. 2011.