Proposal for a modified attenuated total reflection (ATR)-FTIR system

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Chronic kidney disease affects 26 million Americans annually, and is often associated with comorbidities such as diabetes and hypertension [1]. In more recent years, IR spectroscopic analysis of biomarkers, including glucose and certain types of proteins, has become a popular tool in biomedical diagnostics. While testing glomerular filtration rate remains the ideal way to test overall renal function, we want to investigate changing concentrations of biomarkers in biological fluids during haemodialysis as possible diagnostic tools [2]. Previous work has shown that molecules, such as proteins and glucose, have resonant features in the mid-IR [2]. We will use a quantum cascade laser (QCL)-based technology to detect glucose in the mid-IR with the eventual goal of developing a real-time continuous flow biomarker analysis model similar to that found in urine filtrate output during renal dialysis. For proof-of-concept, we are using a Fourier Transform Infrared spectrometer (FTIR) modified to take an attenuated total reflectance (ATR) measurement.

In order to investigate ATR-FTIR spectroscopy as a viable method for measuring glucose concentrations in a free-flowing biological fluid, we evaluated the implementation of a ZnSe prism. Attempting to make a more compact and cost-effective system, we have designed a modified ATR set-up in which the prism is supported from below (Fig. 2). Without utilizing mirrors (as is used in commercially available ATR-FTIR products), the light passes through the crystal using the angles calculated by Snell's Law to obtain attenuated total reflection measurements, and have the sides cut down to an angle of 55^o from the top. This angle was computed by looking at the angle of incidence of the IR light to the side of the prism (see Fig. 1). Using 30^o as angle α, we found angle β to be 11^o. This gave us angle γ, which needs to be larger than the calculated critical angle of 30.66^o in order to obtain total internal reflection. Work supported in part by MIRTHE (NSF-ERC).

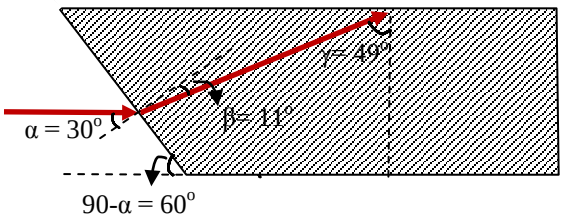

Fig. 1: In order to determine the optimum angles for a modified ZnSe prism, angles were found using the following derivation of Snell's Law: Given 90- (α+β) = γ, and β= arcsin (n_1/n_2 sin(α)), where n_1= 1.00 for air, and n_2= 2.62 for ZnSe.

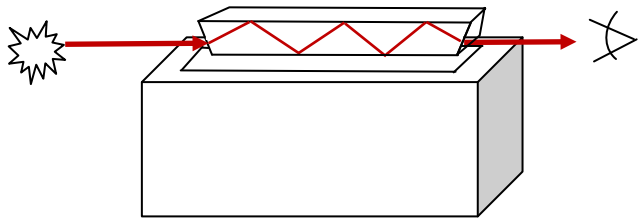

Fig. 2: This is the proposed modification to the traditional ATR-FTIR set-up, which normally utilizes two sets of mirrors. Here, the ZnSe prism can rest directly on a solid base, allowing the light to penetrate the crystal from the right side, and exit the crystal to be picked up by the detector on the left.

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[2] Lopez-Giacoman, Salvador. "Biomarkers in Chronic Kidney Disease, from Kidney Function to Kidney Damage." *World Journal of Nephrology WJN*4.1 (2015): 57-73. Web. 06 July 2016.

[3] Oliver, Katherine V., et al. "Attenuated Total Reflection Fourier Transform Infrared (ATR-FTIR) Spectroscopy as a Bedside Diagnostic Tool for Detecting Renal Disease Biomarkers in Fresh Urine Samples." *Optical Diagnostics and Sensing XV: Toward Point-of-Care Diagnostics* (2015): n. pag. *SPIE Digital Library*. Web. 08 July 2016.