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# The Development of the Python Package PDielec Over the Past 10 Years

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***Abstract*—PDielec is a python package, originally developed as a tool to easily compare calculated infrared and terahertz spectra of powdered, crystalline materials calculated using various density functional theory based packages. This has been continually extended over the past decade with its focus to improve the comparison between calculated and measured spectra.**

## I. INTRODUCTION

PDielec was originally developed as a tool to easily and fairly compare calculated infrared and terahertz (THz) spectra of crystalline materials calculated using various density functional theory (DFT) based packages. This quickly extended to understanding the influence of sample environment on spectra, with a focus on powdered samples, first with the addition of effective medium theories, including both particle shape and size, before extending to both particle scattering and scattering of air inclusions [1]. At the same time the package went through a complete re-write with the inclusion of a GUI and tools for structure and phonon visualization and analysis [2]. More recently, the code has begun to focus on spectra of orientated crystals and crystalline films, for this the code implements transfer and scattering matrix methods to determine the optical behavior of multilayered frequency-dependent films, sandwiched between a superstrate and a substrate. This includes several methods to explore incoherence owing to defects in the crystal or at the interfaces, along with the scattering matrix approach which deals with numerical instabilities when the layers become optically thick. Finally, the package has been restructured with the inclusion of both an API interface and 'experimental' reader. The first makes the code easier to access and extend beyond its original scope as an interface for DFT packages, with this in mind the 'experimental' reader provides an easy way to read other dielectric data such as experimental data or simple model data including four-parameter semi-quantum (FPSQ) [3] or Drude-Lorentz models into the package for further post-processing.

## II. RESULTS

As an example of the capabilities of the single crystal tools available in version 8.2.0 of PDielec, Fig. 1 shows the real and imaginary permittivity of an L-Alanine crystal along each axis of the unit cell, determined from a CRYSTAL14 [4] based calculation performed on a single unit cell. This clearly highlights that orientation of a single crystal or crystalline film will have a significant effect on the measured spectra. Fig. 2 then demonstrates how the optical properties of the material shown in Fig. 1 can be included in an optical propagation model to determine the resultant spectra of a suitable sample. In this case an optical propagation model has been constructed of a 3-layer system with a 200 µm thick crystal of L-Alanine surrounded by air on both sides. The crystal is orientated so that the incident infrared/terahertz beam is perpendicular to the(001) face of the crystal with the azimuthal angle set to 0°.

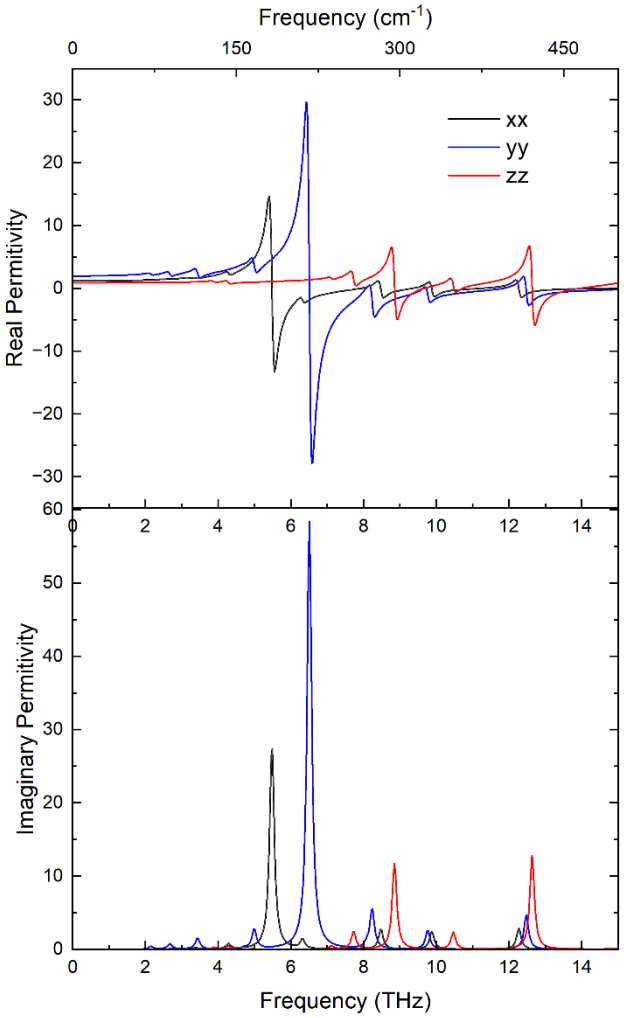


**Fig. 1.** Shows the calculated permittivity along the three different crystalline axis of an L-Alanine Crystal.

Two different propagation models are used and compared, namely a transfer matrix [5] and scattering matrix model [6]. Unfortunately, the transfer matrix method is known to exhibit serious numerical instabilities when the layers become optically thick which leads to the spikes either side of 6 THz in Fig. 2. The scattering matrix method remains numerically stable, even for much thicker samples. This is particularly import as samples far thicker than this have been measured successfully [7] often owing to the large dynamic range of many THz instruments making the scattering matrix methodology particularly useful when comparing to experimental results of real samples.

Fig. 3 shows a similar calculation for the (001) face of MgO based on a DFT calculation using CASTEP [8]. Here the sample is 10 µm thick and the transfer matrix method with air substrate and superstrate is used to determine the light propagation properties of the material. The black curve shows the fully coherent calculation, where the oscillations in the plots are

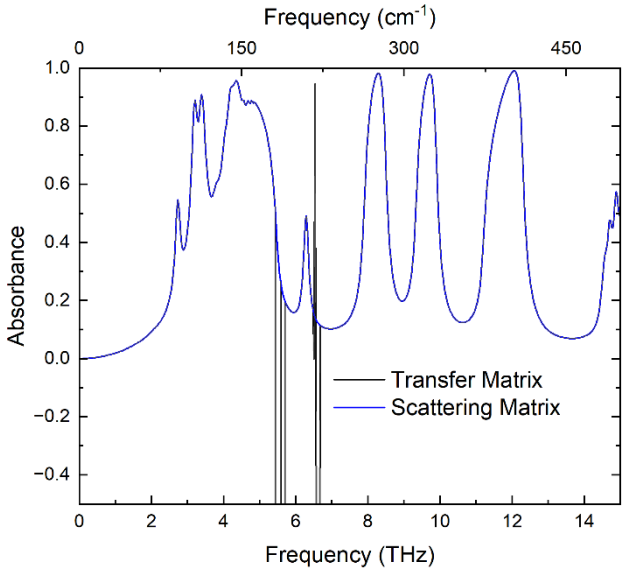


**Fig. 2.** Shows the calculated Absorbance for P-polarised light for an L-Alanine Crystal with light incident on the 001 face of the crystal. Calculations are performed with the Transfer and Scattering Matrix methods.

caused by Fabry–Pérot etalons within the sample. Experimentally, for thick crystals, it is known that the presence of defects in the crystal and at the interfaces, along with variation in sample thickness can cause this coherence to be lost. The blue trace uses the incoherent (phase averaging) method, incorporated within PDielec which is implemented for both transfer and scattering matrix formalisms, and averages over the phase of the propagating matrix for the backward travelling waves in the incoherent material. PDielec incorporates several methods to explore incoherence, including API access to methods to approximate partial coherence which may be necessary when comparing to measurements of optically thick samples in a focused beam as is common place in THz time-domain spectral measurements.

## III. Summary

PDielec has seen significant development over the past decade with recent developments focusing on the incorporation of methods to calculate the spectral response of single crystals and crystalline films. The recent API provision provide access to many of these features.

## AUTHOR CONTRIBUTIONS

A. D. Burnett: Writing — original draft, Investigation; Conceptualization; Methodology; Visualization; J. Kendrick: Writing — review & editing; Investigation; Conceptualization; Methodology; Visualization;

## DATA AVAILABILITY STATEMENT

The example data and code associated with this paper is openly available from [9] with the latest release (v 8.2.0) available from [10].

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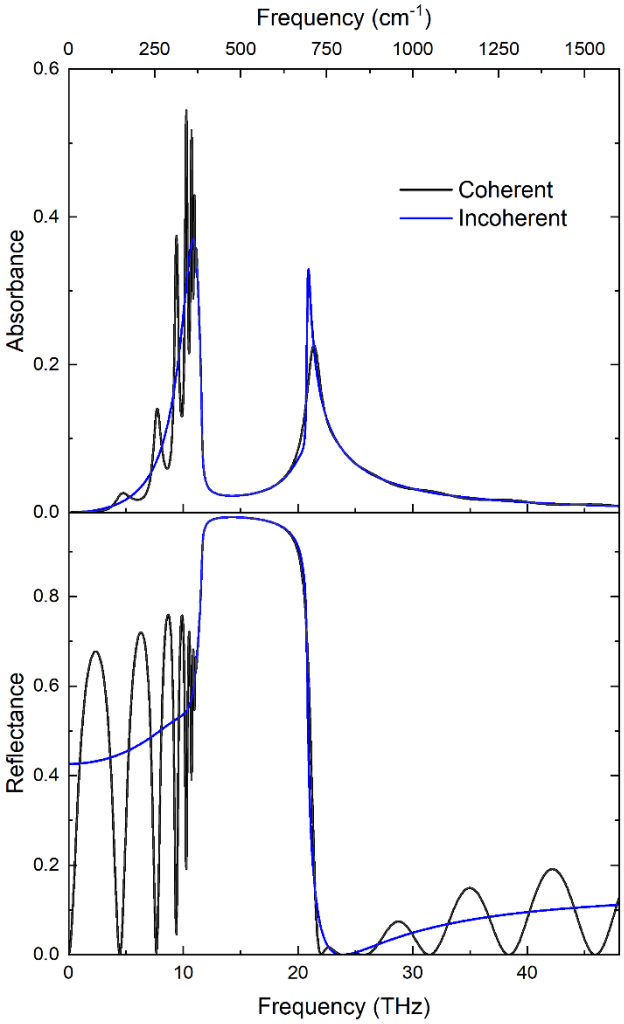


**Fig. 3.** Shows the calculated Absorbance and reflectance for P-polarised light for an MgO Crystal with light incident on the (001) face of the crystal. Calculations are performed with the Transfer Matrix formalism for both a coherent and incoherent (phase averaging) method that prevents etalons within the MgO crystal.

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