White Paper March 10, 2010

Bragg's Law in the Terahertz Regime: Application in Depth Concentration Gradient Estimation

Background

While the Bragg's law is primarily used to determine the lattice spacing of crystalline materials via X-ray diffraction, a macroscopic view of the Bragg's law can be used to obtain a guide line for T-ray usage for scanning across the depth of a substrate. Since T-rays can penetrate most substrates, this provides a unique ability to interrogate the sub-surface in a non-destructive fashion. Fig. 1 shows a plot of the Bragg's law for different terahertz frequencies (wavelengths). It can be seen that not all terahertz frequencies can be used to scan all thicknesses. For smaller thickness, higher terahertz frequency and lower angle of incidence are required. For instance, if one has a source with 3 THz, then at an incident angle of 30° one can only scan a thickness of ~300 μm. In practice, one may want to scan a thinner object and yet keep the angle of incidence smaller so that maximum terahertz radiation will be reflected in to the detector. From this point of view, higher terahertz frequency is desirable.

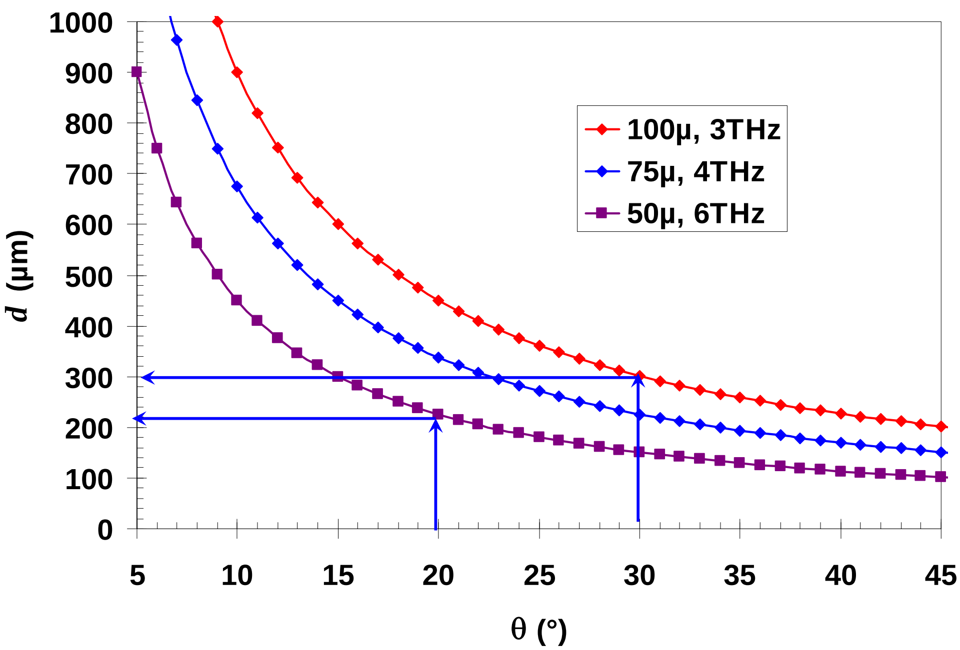

Fig. 1. Plot of Bragg's law for different THz frequencies. Assuming ***d*** is the thickness of the substrate, an angle incidence, θ, can be selected for the reflectance measurement.

In this white paper we show examples of scanning across the thickness of a couple of substrates that provides a means of quantifying the concentration of an active ingredient penetrated through the thickness of the given substrate. A calibration can be established for a given substrate for different concentrations of an applied active ingredient. Such calibration can be used for subsequent determination of unknown concentration at a given depth. The technique can be further developed for sub-surface spectral analysis and imaging.

Experimental

Fig. 2 shows a sketch of a setup that can be used for scanning a substrate across its thickness for detecting and quantifying reagents that may have penetrated with an effective concentration gradient. A procedure need to be established to obtain the concentration from the measured reflected power. First, a scan of the blank substrate is made as the reference. Then the reflectance is measured after the reagent is applied and the solvent (if any) is dried. The difference of these two measurements is assigned to the net absorption of the reagent by the substrate material. Thus, measurements of known concentration gradient will serve as a calibration curve for determining unknown concentration at a given depth of a given substrate.

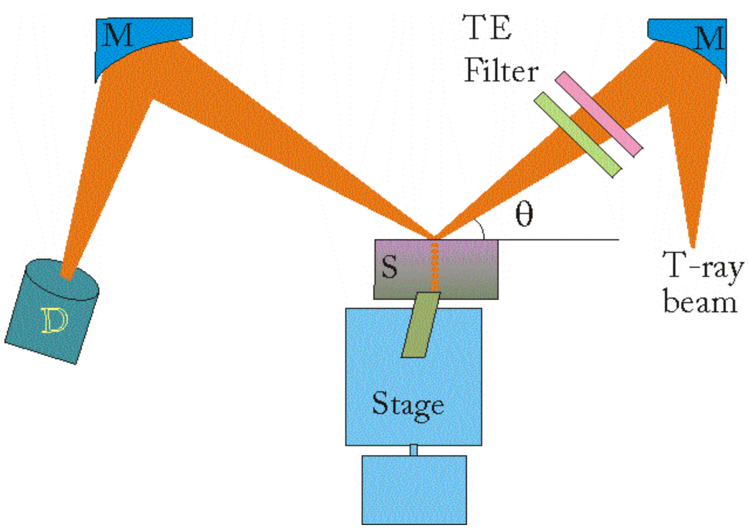

Fig. 2. Experimental setup for characterizing concentration gradient across the depth of a substrate. The angle of incidence should be selected based on the thickness of the substrate and in accordance with the Bragg's law shown in Fig. 1.

Examples of application

The principle was applied to substrates of different compositions. Fig. 3 shows an example of Ceraphyl RMT penetration in a cardboard. The power difference between the blank cardboard and 100% Ceraphyl treated cardboard, Delta, is a measure of Ceraphyl concentration across the thickness. Calibration should be conducted a priori for a given substrate for different known concentrations to establish the penetration behavior. From such calibration unknown concentration at a given depth can be estimated. Examining Fig. 3 (red curve) it can be surmised that over up to ~100 µm the penetrated Ceraphyl concentration is approximately unchanged, but from 100 µm to ~450 µm concentration falls gradually reaching the lowest at ~450 µm. The cardboard being highly porous, the penetration behavior observed from Fig. 3 is reasonable. While from 450 µm to 600 µm slight increase in the power is observed, this is probably due to the fact that a mirror is placed on the back of the card. This mirror is used to

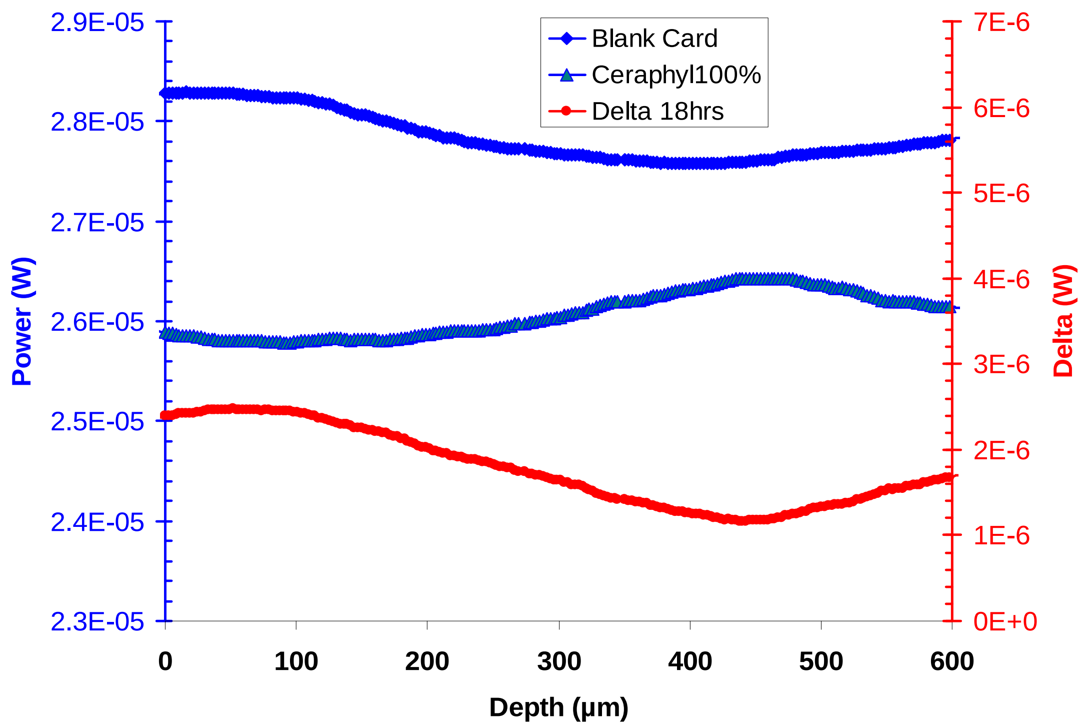

Fig. 3. Penetration of Ceraphyl RMT across the depth of a cardboard. The blank cards profile is (top curve, blue diamond) compared with the profile of the same card but treated with 100% Ceraphyl RMT, dried overnight (middle curve, blue triangles). The difference of the blank and Ceraphyl treated card is assigned to Ceraphyl concentration across the thickness of the card (bottom curve, red circles, right Y-axis).

determine the focal point of the THz radiation so that the substrate front surface can be positioned at the focal point. Subsequent measurements can be done without the mirror; however, it was not removed from the present setup.

Another example is shown in Fig. 4. Here a piece of plank (porous, single layer wood) was used as substrate and it was treated with a methanolic solution of Ceraphyl RMT (4.619 mg/ml). The plank was dried over night at room temperature. Unlike the previous cardboard example, here the Ceraphyl treated plank has a higher reflection compared to untreated substrate. This is characteristic of differences in the material of a given substrate compared to other substrate materials. However, there is a clear difference in the reflected power between the treated and untreated plank that is used to calculate the Delta corresponding to the penetrated Ceraphyl. It is also seen that the Delta (red curve, right Y-axis of Fig. 4) for the lower Ceraphyl concentration is significantly smaller compared to the Delta of 100% Ceraphyl (Fig. 3). This indicates that, once calibrated, the method will be independent of the substrate material.

Summary

In this white paper we outline a technique for determining the concentration gradient across the thickness of a substrate when an active ingredient is applied and that has penetrated through the surface. The method provides a direct measurement of the depth profiling without requiring any complementary experiments. Compared to other methods such as small angle X-ray scattering or small angle neutron scattering that require dedicated facility and huge budget, this is a robust yet very cost-effective method. It is simple enough to be carried out by trained technician and can be deployed for day-today quality control purposes as well as for research applications. With further development this method can also be used for under the surface imaging and spectral characterizations.

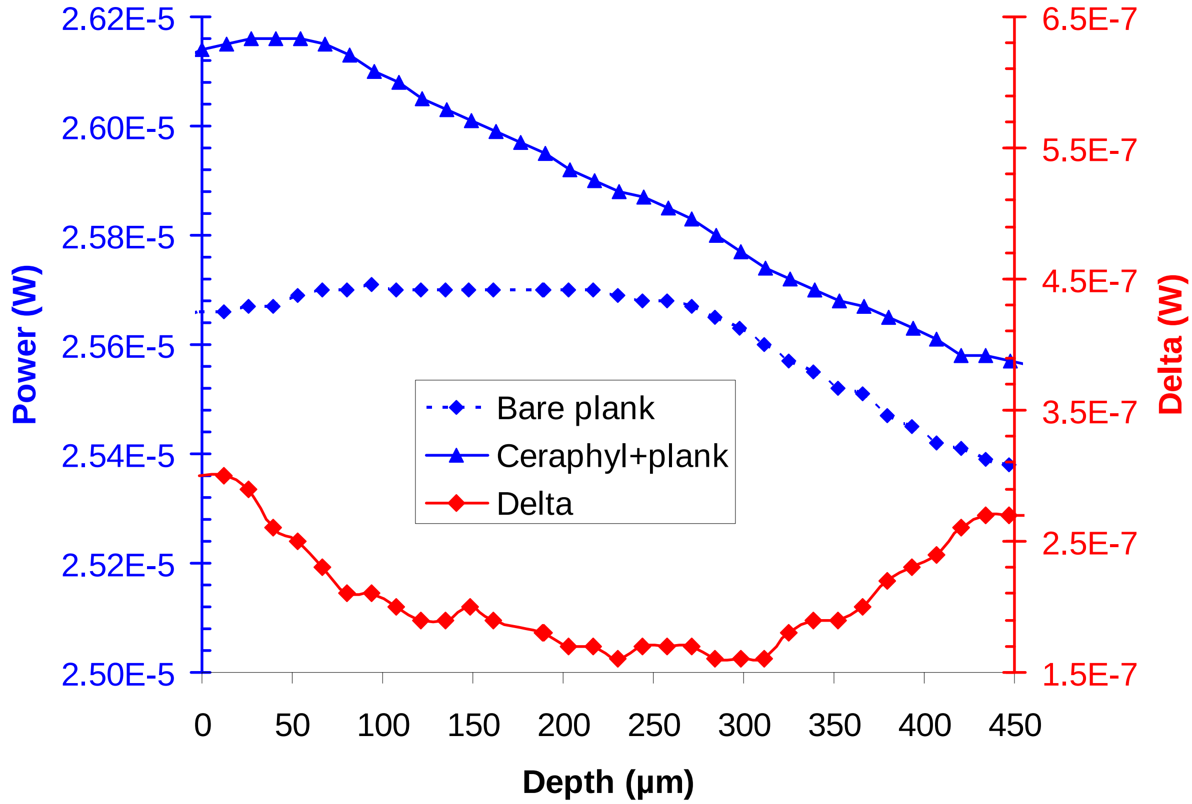

Fig. 4. Penetration of Ceraphyl RMT across the depth of a small plank (porous, single layer wood). The blank plank profile is (middle curve, blue diamonds) compared with the profile of the same plank but treated with 4.619 mg/ml Ceraphyl RMT solution in methanol, dried overnight (top curve, blue triangles). The difference of the blank and Ceraphyl treated plank is assigned to Ceraphyl concentration across the thickness of the plank (bottom curve, red diamonds, right Y-axis).

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