Accounting for the pellet's porosity in THz-TDS measurements of powder oxides

Jaume Calvo-de la Rosa[1,2], Alexandre Locquet[2,3], Denis Bouscaud[4], Sophie Berveiller[4], and D.S. Citrin[2,3]

[1] *Department of Condensed Matter Physics, Faculty of Physics, IN2UB, Universitat de Barcelona, Martí i Franquès 1, 08028, Barcelona, Spain*

[2] *Georgia Tech-CNRS UMI 2958, Georgia Tech Lorraine, 2 Rue Marconi, 57070, Metz, France*

[3] *School of Electrical and Computer Engineering, Georgia Institute of Technology, Atlanta, GA, 30332-0250, USA*

[4] *Laboratoire d'Etude des Microstructures et de Mécanique des Matériaux LEM3 (UMR CNRS 7239), Arts et Métiers ParisTech, Université de Lorraine, 4 rue Augustin Fresnel, 57078, Metz, France*

Corresponding author: jaumecalvo@ub.edu

Terahertz time-domain spectroscopy (THz-TDS) is every time a more popular technology to study the optical and dielectric properties of materials in the THz frequency range, typically from 0.1 THz to 10 THz. Materials such as explosives, drugs, organic, ceramic or composites are commonly studied by THz-TDS. However, due to the high attenuation that many of these materials have, it is common to work with powder materials dispersed into a THz-transparent matrix (typically polyethylene, PE).

Despite this is a very common practice, the experimental implementation needs to be carefully done and requires a detailed interpretation of the data in order to avoid other effects to appear, leading to an error on the property's deduction. Some of these non-intrinsic effects are size dependencies (i.e., powder – bulk different behaviour), the relative volume between powder and matrix (known as *filling factor*, f_v), scattering, or percolation between particles, for instance. Many of these effects can be accounted by using Effective Medium Models (EMMs), which are commonly used to extract the pure powder's properties from the measured properties of the mixture.

Nonetheless, the porosity contained inside the pellet (within the PE matrix, for instance) is not considered by the EMMs and it is often forbidden in THz-TDS works. However, if the porosity level is high, this might have an important effect on the measured properties due to the large permittivity difference between air and the powder materials typically investigated. In this work we propose a methodology based on a sequential two-step' implementation of EMMs to quantify the contribution of the porosity on THz-TDS measurements on CuO and ZnO powder samples.

Our algorithm considers the pellet as a ternary system (powder + PE + air) instead of a binary one (powder + PE). Contrary to previous works, which solve this problem by applying three-phases implementations of a single EMM (such as Maxwell-Garnett or Bruggeman), our approach is capable to adapt to each phase physical characteristics and uses a specific model for each phase. Our results show very good agreement between experimental data and models and conclude that the most accurate results are obtained by using a combination of the Vegard's law (to account for the porosity) and the Maxwell-Garnett model (to deduce the oxides' properties).

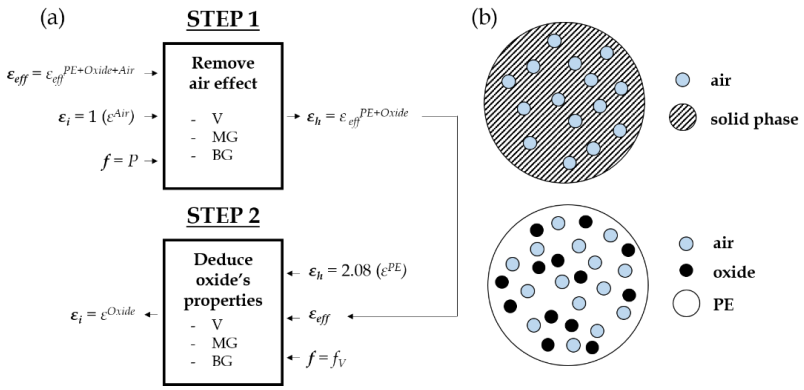

Fig. 1: Scheme of the developed two-steps method based on the combination of two EMMs. Fig. from [2].

References:

[1] J. Calvo-de la Rosa, *et al*., Ceramics International 46 (15), 24110-24119 (2020).

[2] J. Calvo-de la Rosa, *et al*., IEEE Trans. Terahertz Sci. Technol. Early Access (2021).