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Jonathan Breeze

Temperature and Frequency Dependence of Complex Permittivity in Metal Oxide Dielectrics: Theory, Modelling and Measurement

Doctoral Thesis accepted by
London South Bank University, London, UK

Springer

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Supervisor's Foreword

In the past few decades there has been an explosion in satellite and mobile telecommunications technology. It is estimated that there are now more mobile phones than there are people on the planet. Microwave communications for voice, images, data and music are also closely correlated with the gross domestic product of a nation so the importance of the technology cannot be overstated. Microwave dielectrics play a key role in the development of the technology. Dielectric resonators are able to act as tuning forks; when an electromagnetic wave interacts with a dielectric the material resonates. Furthermore the wavelength of the electromagnetic waves can be "compressed" to be much shorter than the free space wavelength, permitting miniaturisation that is proportional to the reciprocal of the material's relative permittivity. The length of time that the resonator can "ring" once it has been struck with the electromagnetic wave is known as the quality factor or 'Q'. The Q is a measure of the material's dielectric loss and it is crucial that the loss be as low as possible. Finally the temperature coefficient of the dielectric constant (sometimes expressed as the temperature coefficient of frequency) is the third important parameter. Here, these three parameters are explored from the viewpoint of both theory and experiment.

Historically, the dielectric loss in particular has proven exceptionally difficult to describe, and the best theories so far have unfortunately been physically correct but practically unsatisfactory as they have been unable to predict the microwave dielectric loss in real materials that contain defects—all materials contain defects.

The thesis explores metal oxide based microwave dielectric ceramics, important materials in radio, microwave and terahertz applications. The performance of devices using these materials are often limited by absorption of electromagnetic energy or dielectric loss, which has been described theoretically as due to anharmonic coupling between lattice vibrations (phonons). Quantum field theory had been applied successfully to develop a theory of loss, yet absolute values of predicted losses were often orders of magnitude different to measurements. Historically, this was due to a lack of accurate data on the lattice dynamical properties of metal oxides and needing to resort to empirical models of

anharmonicity. This thesis shows for the first time that a theory of anharmonic phonon coupling using results from density function perturbation theory can predict from first principles the complex permittivity of metal oxides as a function of temperature and frequency. Here, the temperature and frequency dependence of relative permittivity and loss for MgO were calculated and found to be in excellent agreement with microwave measurements and terahertz spectroscopy. These results provide insight into the mechanisms of dielectric loss in oxides and offer the opportunity of engineering better dielectrics, especially for the rapidly developing terahertz field where losses are important.

The work was supported by the Engineering and Physical Sciences Research Council.

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Prof. Neil McN. Alford

Abstract

This thesis investigates the dielectric properties of metal oxide ceramics at microwave frequencies. Dielectric ceramics are an important class of material for radio frequency, microwave and emergent terahertz technologies. Their key property is the complex permittivity, its real part permits miniaturisation of devices and its imaginary part is responsible for absorption of electromagnetic energy. Absorption limits the practical performance of many microwave devices such as filters, oscillators, passive circuits and antennas. The complex permittivity as a function of temperature for low-loss dielectrics is determined by measuring the resonant frequency of dielectric resonators and using the radial mode-matching technique to extract the dielectric properties.

There have been only a handful of publications on the theory of dielectric loss whose predictions have often been unfortunately unsatisfactory when compared to the measurements of real crystals, sometimes differing by orders of magnitude. The main reason for this is the lack of accurate data for anharmonic coupling coefficients and phonon eigenfrequencies at arbitrary q vectors in the Brillouin zone.

Here, a quantum field theory of losses in dielectrics shall be applied using results from density functional perturbation theory, to predict from first principles the complex permittivity of metal oxides as functions of frequency and temperature.

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