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Fundamental mechanisms that determine the loss tangent and temperature coefficient of resonant frequency (τf) in modern microwave ceramic dielectrics

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Despite the practical importance of achieving a small loss tangent (tan δ) and near-zero temperature coefficient of resonant frequency (τF) for microwave communication systems, a fundamental understanding of which mechanism determine these important parameters had not been firmly established. In this talk, I will focus on my group's work using modern experimental and theoretical condensed matter methods to identify the responsible mechanisms. We will focus our discussions on results from Ni-doped BaZn-Ta2/3O3 (BZT), since it is the highest performer at room temperature. We will also show that the conclusions are general for other commonly-used materials. Ba(Zn1/3Ta2/3)O3 exhibits the unusual combination of a large dielectric constant, ε_r, and a small loss tangent at microwave frequencies. Using ab-initio electronic structure calculations, we show that d-electron bonding in BZT and related materials is responsible for producing a more rigid lattice with higher melting points, enhanced phonon energies than comparable ionic materials and thus inherently less microwave loss. The properties of commercial materials are optimized by adding dopants or alloying agents, such as Ni or Co to adjust the temperature coefficient, tF to zero. This occurs as a result of the temperature dependence of ε offsetting the thermal expansion. At low temperatures, we show that the dominant loss mechanism in these commercial materials comes from spin excitations of unpaired transition-metal d electrons in isolated atoms (light doping) or exchange coupled clusters (moderate to high doping), a mechanism differing from the usual suspects. At high temperatures, we give evidence that loss also arises and may be dominated by localized hopping transport. The temperature coefficient of resonant frequency (τf) of a microwave resonator is determined by three materials parameters according to the following equation: $\tau f = -(\frac{1}{2}\tau\varepsilon + \frac{1}{2}\tau\mu + \alpha L)$, where αL, τε and τμ are defined as the linear temperature coefficients of the lattice constant, dielectric constant, and magnetic permeability, respectively. We have experimentally determined each of these parameters for undoped and Ni-doped Ba(Zn1/3Ta2/3)O3 materials. These results, in combination with density functional theory (DFT) calculations, have allowed us to develop a nearly complete understanding of the fundamental mechanisms responsible for τf.

Biography

Nathan Newman is a Professor of Solid State Sciences and is a faculty member in the Materials Program at Arizona State University. His research interests focus on the investigation of novel solid-state materials for microwave, photonic and high-speed applications. His current work involves synthesis, characterization and modeling of novel superconductor junctions and materials, III-N semiconductors, low loss dielectrics for microwave communication, and novel photovoltaic material. He is an author and co-author of over 200 technical papers, has 12 patents, has an h-index over 40 and his papers have been cited over 5,000 times. He has received the *IEEE Van Duzer Award, is a Fellow of the IEEE and the American Physical Society*, and has won Faculty Teaching Awards at Northwestern University and Arizona State University. He also serves as an Associate Editor for Materials in the *IEEE Transactions of Applied Superconductivity* and has served as the Chair of the US Committee on Superconductor Electronics and ASU's LeRoy Eyring Center for Solid State Sciences.

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