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Mechanism for dielectric loss and temperature dependence of dielectric constant (ϵ) in modern microwave materials

Despite the practical importance of low-loss temperature-compensated microwave ceramics for next-generation communication systems, a quantitative understanding of what determines the loss tangent and temperature dependence of the dielectric constant (ϵ) have not been firmly established. We focus our discussions on Ni-doped $\text{BaZn}_{1/3}\text{Ta}_{2/3}\text{O}_3$ since it is the highest performer at room temperature and show that our conclusions are general for other commonly-used materials. $\text{Ba}(\text{Zn}_{1/3}\text{Ta}_{2/3})\text{O}_3$ exhibits the unusual combination of a large dielectric constant, ϵ_r and a small loss tangent at microwave frequencies. Ab-initio electronic structure calculations show this desirable property from the “covalent” charge transfer between the cation d-orbitals (from Ta 5d-levels at CBM to Zn 3d-levels at VBM); providing a degree of covalent directional bonding that resists angular distortions between atoms, resulting in a more rigid lattice with enhanced phonon energies and thus inherently low 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, τ_F to zero. This occurs as a result of the temperature dependence of ϵ_r off-setting 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. Temperature- and magnetic-field dependent measurements of the lattice constant, microwave loss and dielectric constant, in combination with density-functional theoretical modeling, give evidence of the direct role of localized hopping transport on loss and phonon-induced structural changes on dielectric constant at higher temperatures.

Biography

Nathan Newman serves as the Lawrence Professor of Solid State Sciences and is a faculty member in the Materials Program at Arizona State University. His current work involves synthesis, characterization and modeling of novel superconductor junctions and materials, III-N semiconductors, low loss microwave dielectrics and novel photovoltaic material. He has authored or co-authored over 200 technical papers and 12 patents. He received the IEEE Van Duzer award and is a Fellow of the IEEE and the American Physical Society. He serves as an Editor for Materials in the IEEE Trans. of Appl. Superconductivity and has served as Chair of the US Committee on Superconductor Electronics and ASU's LeRoy Eyring Center for Solid State Sciences.

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