Chemical/Displacive Ordering in Complex Perovskites

Igor Levin
Ceramics Division, NIST, Gaithersburg MD USA
igor.levin@nist.gov

Complex $A(B'_{1/3}B''_{2/3})O_3$ perovskites display a variety of interesting properties. For example, some of these compounds exhibit relaxor ferroelectric behavior, while others feature low dielectric losses and serve as dielectric resonators in wireless communication systems. Additionally, non-stoichiometric $A(B'_{1/3+x}B''_{2/3-x})O_{3-y}$ perovskites exhibit ionic conductivity and can also absorb significant proton concentrations becoming proton conductors. The common crystal-chemical effects operating in these compounds include B-cation ordering and/or structural distortion approximated by rotation of nearly rigid $[BO_6]$ octahedra; both effects are known to have a strong effect on dielectric and electrical properties. The chemical ordering is largely driven by the B-cation size mismatch, while the driving force for the octahedral tilting increases with increasing $(R_B - R_A)$ size difference. In this presentation, we will discuss chemical/displacive ordering in the $Ca(Ca_{1/3}Nb_{2/3})O_3$ and $Sr(Sr_{1/3}Nb_{2/3})O_3$ perovskites with large Ca and Sr ions occupying both A- and B' sites. The structural details and phase transitions in these compounds were analyzed using transmission electron microscopy combined with X-ray and neutron powder diffraction.