Ferroelectric (FE) ceramics are now recognized as promising materials for microwave devices due to their high dielectric tunability (ability to change the dielectric constant with applied electric field) and low dielectric loss (caused by leakage currents). The figure of merit for tunable microwave applications can be written as:

\[
\text{Figure of Merit} : K = \frac{\tau}{\tan \delta},
\]

\[
\text{Tunability} : T = \frac{C_{\text{max}} - C_{\text{min}}}{C_{\text{max}}},
\]

\[
\text{loss tangent} : \tan \delta = \frac{\varepsilon_2}{\varepsilon_1},
\]

where \(C_{\text{max}}\) and \(C_{\text{min}}\) are the maximum and minimum capacitance and \(\varepsilon_1\) and \(\varepsilon_2\) are the real and imaginary dielectric constants. The challenge for microwave application is to obtain a material with \(K=100\) at 100 GHz. To obtain maximum performance it is necessary to maximize the tunability and decrease loss at the operating frequencies. The current materials find limited applicability in microwave applications due to the increase of the loss with frequency and (for high quality crystals) bias electric field. We developed a methodology to predict the response of thin film ferroelectrics using a hierarchical modeling chain from QM to the millimeter scale of real ferroelectric films. Application of this methodology found a critical frequency, which corresponding to the maximum energy loss.

Figure 1. Multiscale phenomena of domain wall are simulated by multiscale simulation methods.