Modeling Domains in $PbSc_{1/2}Nb_{1/2}O_3$ using an effective Hamiltonian Approach

ERIC COCKAYNE, BENJAMIN P. BURTON,
Ceramics Division, Materials Science and Engineering Laboratory
National Institute of Standards and Technology,
Gaithersburg, MD 20899, USA
UMESH WAGHMARE
Theoretical Sciences Unit, J. Nehru Center for Advanced Scientific Research
Jakkur, Bangalore, 560064, India

$PbSc_{1/2}Nb_{1/2}O_3$ (PSN) exhibits relaxor behavior over a range of temperatures close to the maximum in its low-frequency dielectric function $\epsilon'(T)$. The dielectric properties of PSN are strongly dependent on the ordering of Sc and Nb and whether or not Pb vacancies (presumably Pb-O vacancy pair clusters) are present. We use a first-principles-based effective Hamiltonian to model the effects of various types of B-site ordering on $\epsilon'(T)$. Specifically, we compare cation configurations which exhibit: (1) perfect fcc order (2) short-range order (3) random disorder and (4) fcc-ordered domains in a random matrix. We also investigate the effect(s) of including enhanced local fields at certain sites, as might be caused by Pb vacancies. For structures with distinct domains, we study the individual contributions of each pair of domains to $\epsilon'(T)$.