# Long range and local structure of $Sr_xBa_{1-x}Nb_2O_6$ (x = 0.33 and 0.67), from room temperature to 720 K

Cheng Li[a] and Yuanpeng Zhang[a]

[a] Spallation Neutron Source, Oak Ridge National Lab, 37830, TN, lic1@ornl.gov , zhangy3@ornl.gov

Tetragonal tungsten bronze (TTB), with the general formula $A'_2A''_4B'_2B''_8O_{30}$, has a flexible chemical framework and offers great opportunity for property tuning by modifying the composition and stoichiometry of the sample [1]. In the well-studied $Sr_{1-x}Ba_xNbO_6$ (SBN) prototype, a drastic change in dielectric response, namely a crossover between normal ferroelectric (FE) response to relaxor (RE) behavior, was obtained when $x > 0.6$ [2]. The FE to RE crossover was interpreted as a result of the enhanced structural disorder with high Sr content [3]. For instance, increasing cation vacancy concentration at A" site was reported to promote structural disorder in SBN [4]. Indeed, various macroscopic metrics, including A'/A" cation ratio and *c*/*a* ratio, have been proposed to characterize the degree of structural disorder [1]. There is however a missing link between the local atomic configuration and the RE to FE transition in TTB phases, although it is well known the local structure is often responsible for varied dielectric response [5].

We therefore investigated long-range and local structure of SBN33 and SBN67, across their paraelectric phase transition, using a combination of Rietveld, small box PDF and RMC methods. We observed diffused scattering background from room temperature up to 720 K, 300 K above their phase transition temperatures (Figure 1a). In addition, abnormal change in the atomic displacement parameters, namely, continuous *decrease* of oxygen ADP with *increasing* temperature, as well as a jump in $U_{33}$ at Nb1 site above $T_c$, points to local static ordering in the TTB system (Figure 1b).

The static local ordering was confirmed with PDF analysis: the centrosymmetric average structure could not model the local structure at 720 K, and the local structure seems to follow the low temperature, non-centrosymmetric space group (Figure 2). The combined PDF and RMC analysis revealed two distinguished Nb local environment: while the polarization in Nb2 sties becomes negligible, the local displacement of Nb1 site is comparable above and below $T_c$. Our model revealed static local ordering involving neighboring $NbO_6$ tilting, which averages out at the macroscopic scale.

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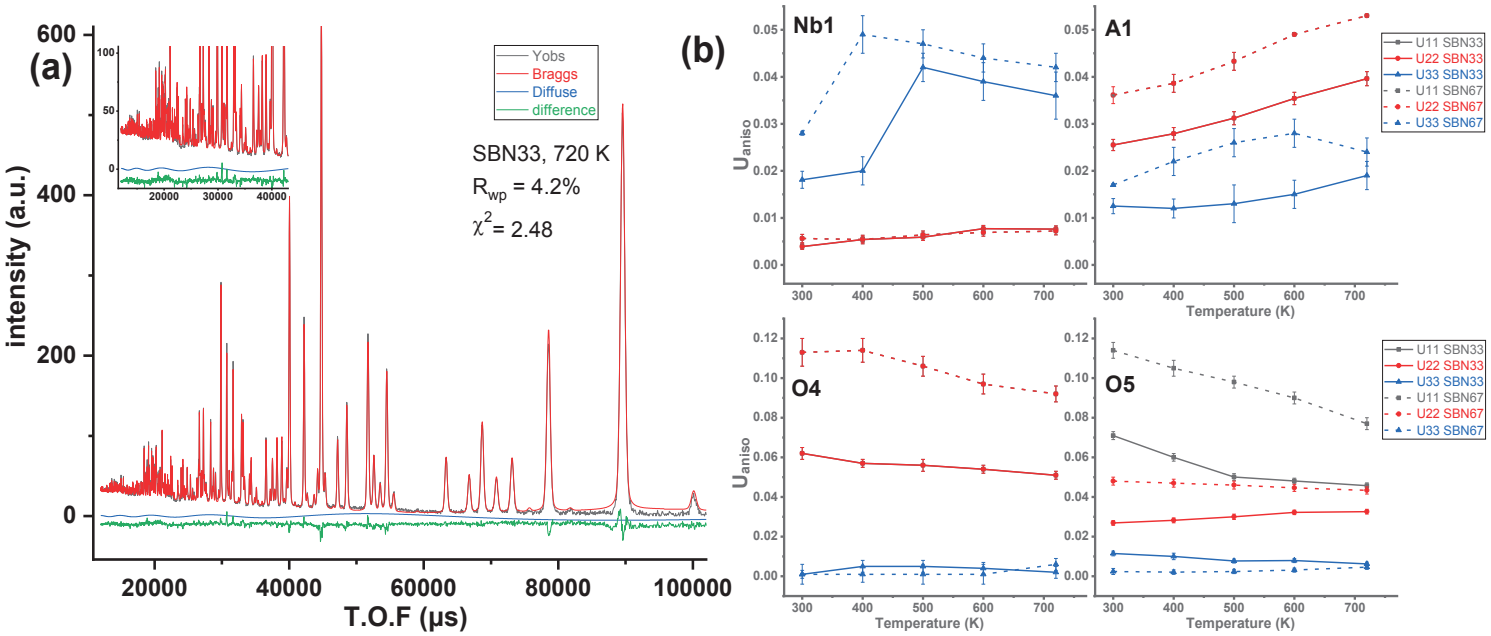


Figure. 1 a) Rietveld refinement of the SBN33 composition at 720 K, a diffused scattering background was observed 300 K above the paraelectric phase transition b) refined atomic displacement parameters from 300 K to 720 K of selected atomic sites, revealing an abnormal change in ADP.

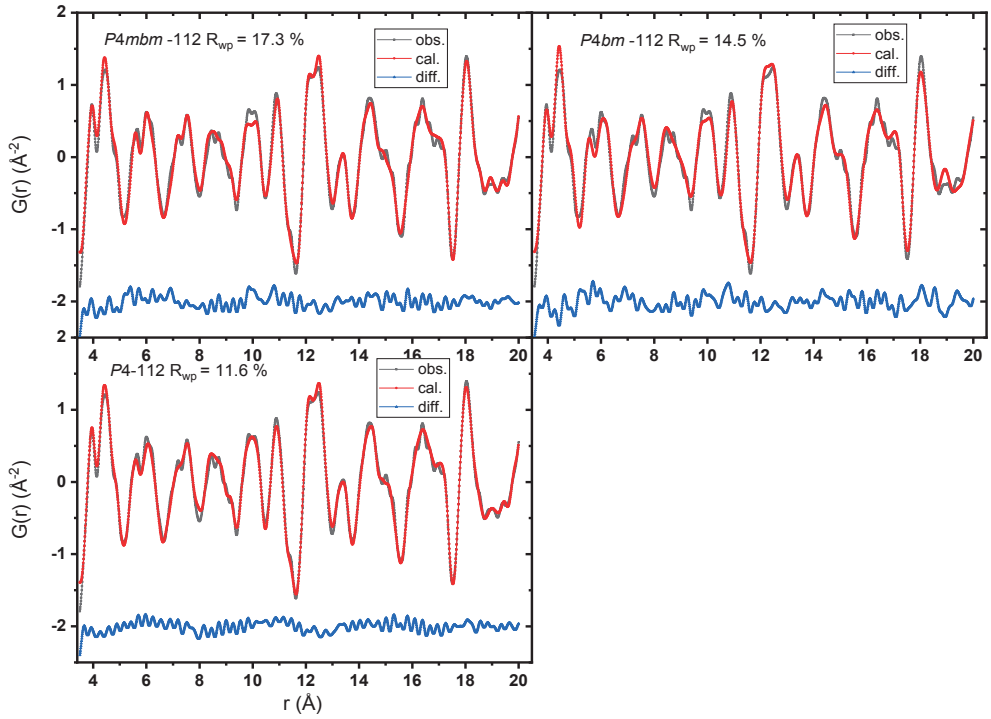


Figure 2. PDF small box fitting of the 700K data of the SBN33 composition. Different space group namely a) paraelectric P4mbm b) low temperature P4bm and c) its subgroup P4 was used. The results indicate a ferroelectric distortion in the local structure