Machine learning analysis of microwave dielectric properties for seven structure types: The role of the processing and composition

Natalia Kireeva[1,2] and Vitaly P. Solovev[1]

[1]Frumkin Institute of Physical Chemistry and Electrochemistry RAS, 31, Leninsky prospect, Moscow, 119071, Russian Federation

[2]Moscow Institute of Physics and Technology, 9 Institutskiy per., Dolgoprudny, Moscow Region, 141700, Russian Federation

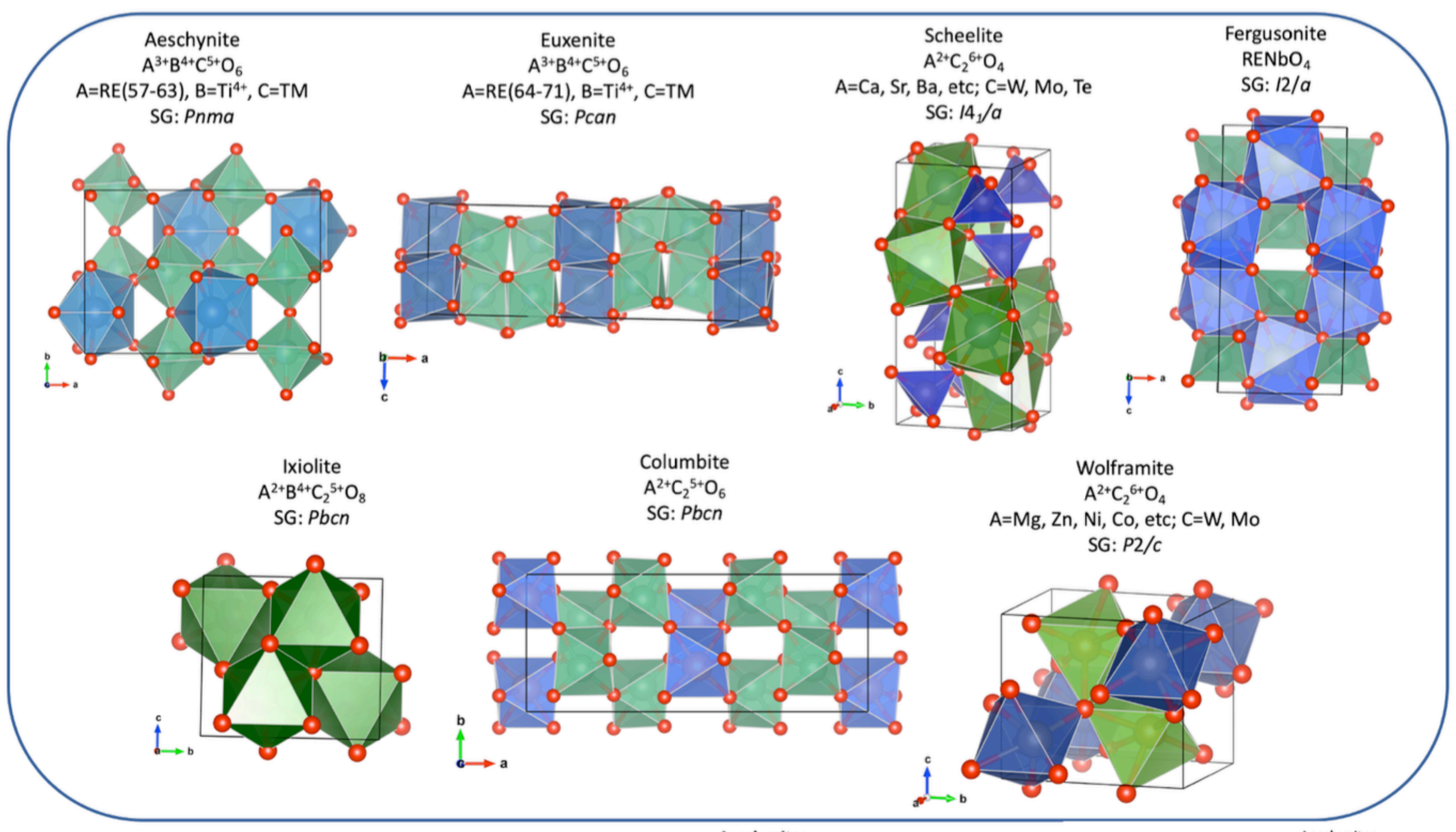
Abstract

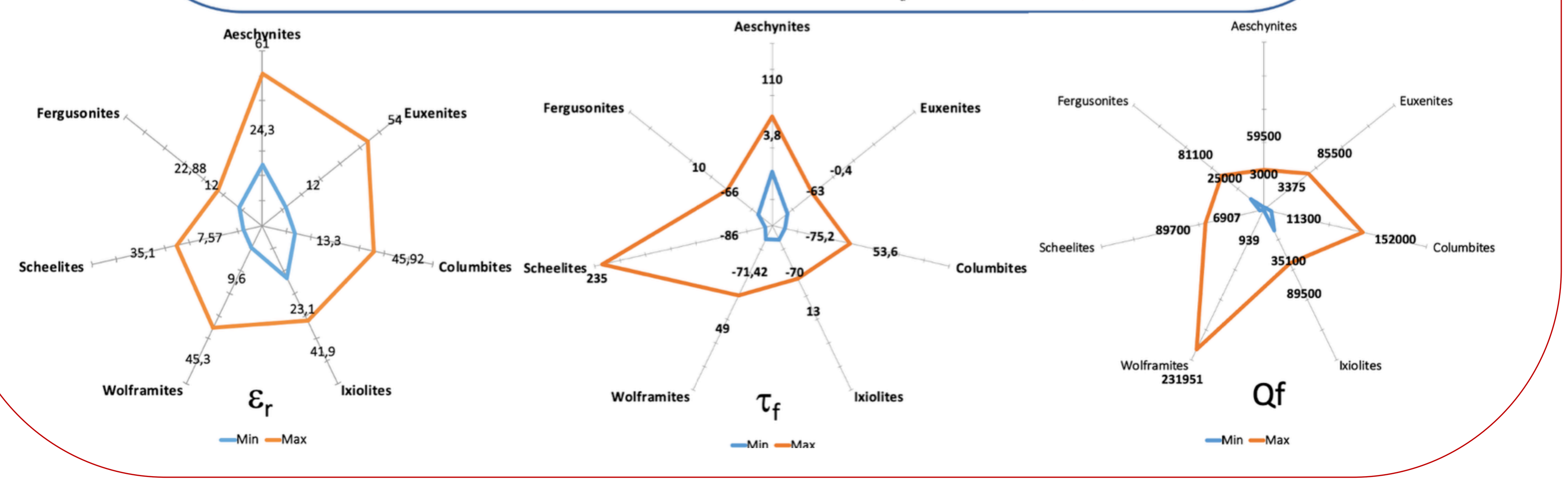
During the last decades the area of wireless communications experienced the drastic growth demanding the search for new materials with tailored microwave dielectric characteristics. Microwave dielectric properties of ceramic materials have been extensively studied, the comprehensive database of microwave dielectric properties is now available [1, 2]. Several studies involving machine learning approaches have been performed [3, 4].

In this study, machine learning approaches have been used for synthesis-structure-property relationships assessment. The analysis has been performed for several structure types. The new descriptors encapsulating the information on the constituent building blocks, their relative number and connectivity have been introduced. These structure-characterizing parameters, the hybrid of descriptors recently proposed in [5] and [6], can be regarded as a flexible way to describe the inorganic crystal structures using the substructural bottom-up approach comprising both, the symmetry and the connectivity information.

The role of the processes observed at the grain boundaries as well as the re-crystallization processes for the microwave dielectric characteristics is discussed. The impact of the heat-treatment and the composition for the considered structure types is discussed. More details of this study can be found in [7].

Data: Structure Types Used for Modeling

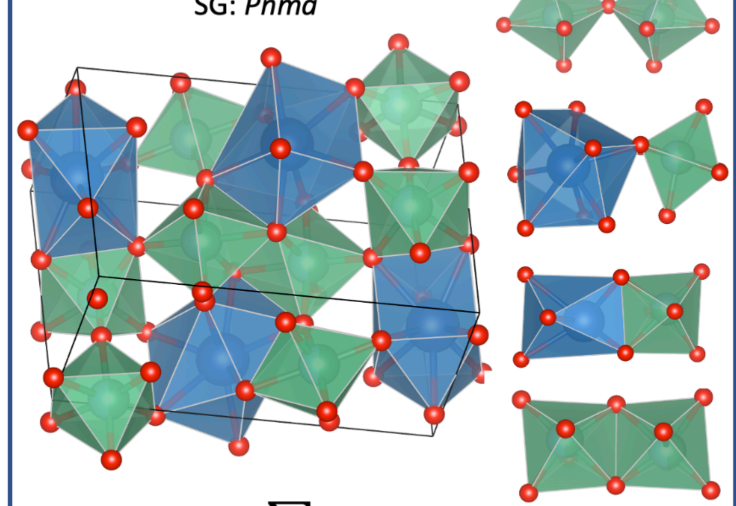




Descriptors

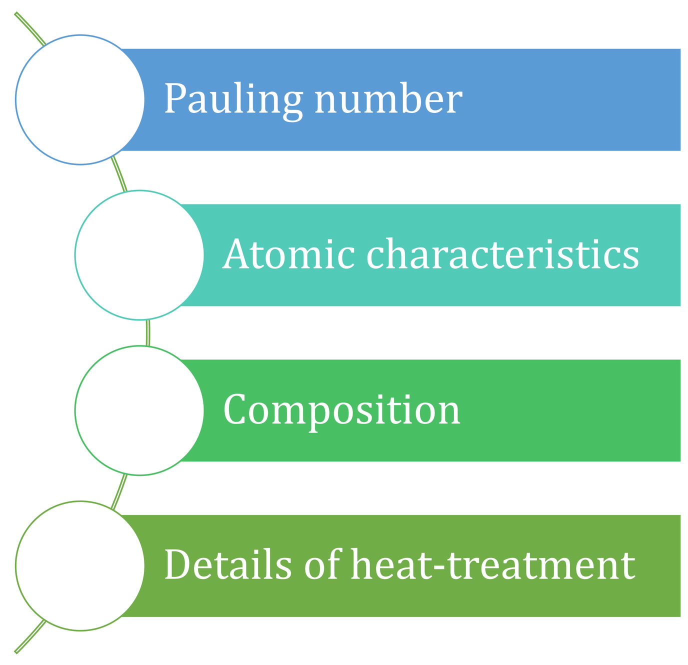
Structure parameter PN

Aeschynite
$A^{3+}B^{4+}C^{5+}O_6$
A=RE(57-63), B=Ti4+, C=TM
SG: Pnma



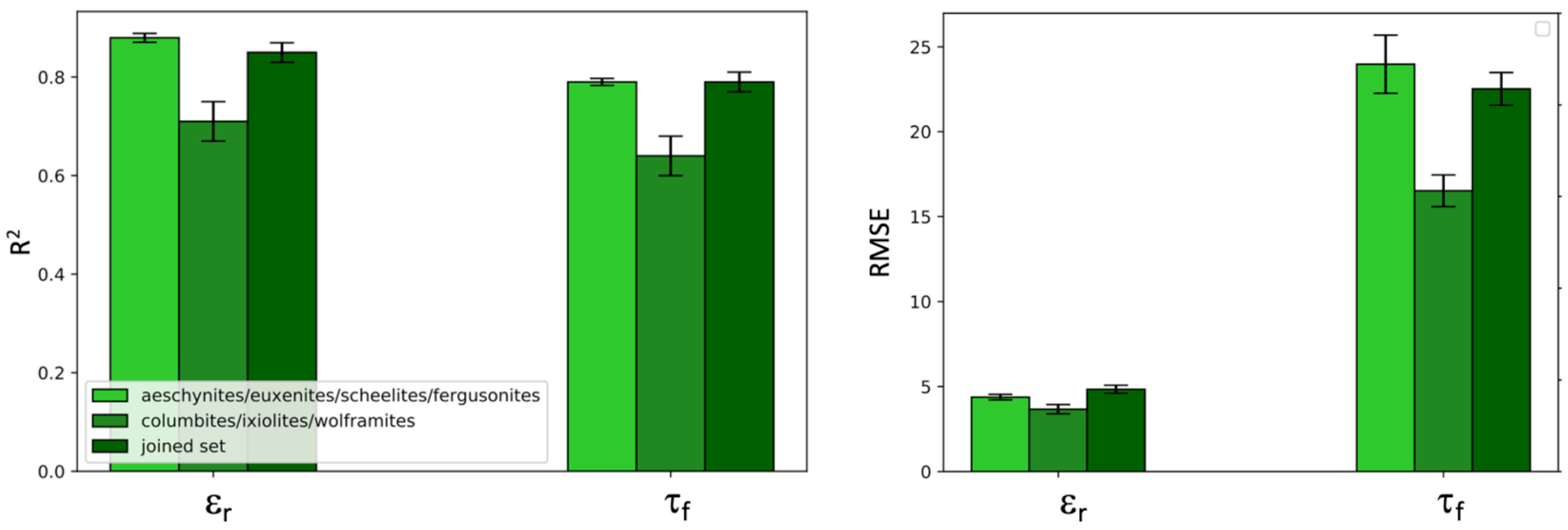
$$PN = \sum_i m_i \cdot n_i / 2^{d+1}$$

m – the relative number of polyhedra connected similarly
n – the order of the point group symmetry of polyhedra
d – the type of connectivity (nodes, edges, grains)

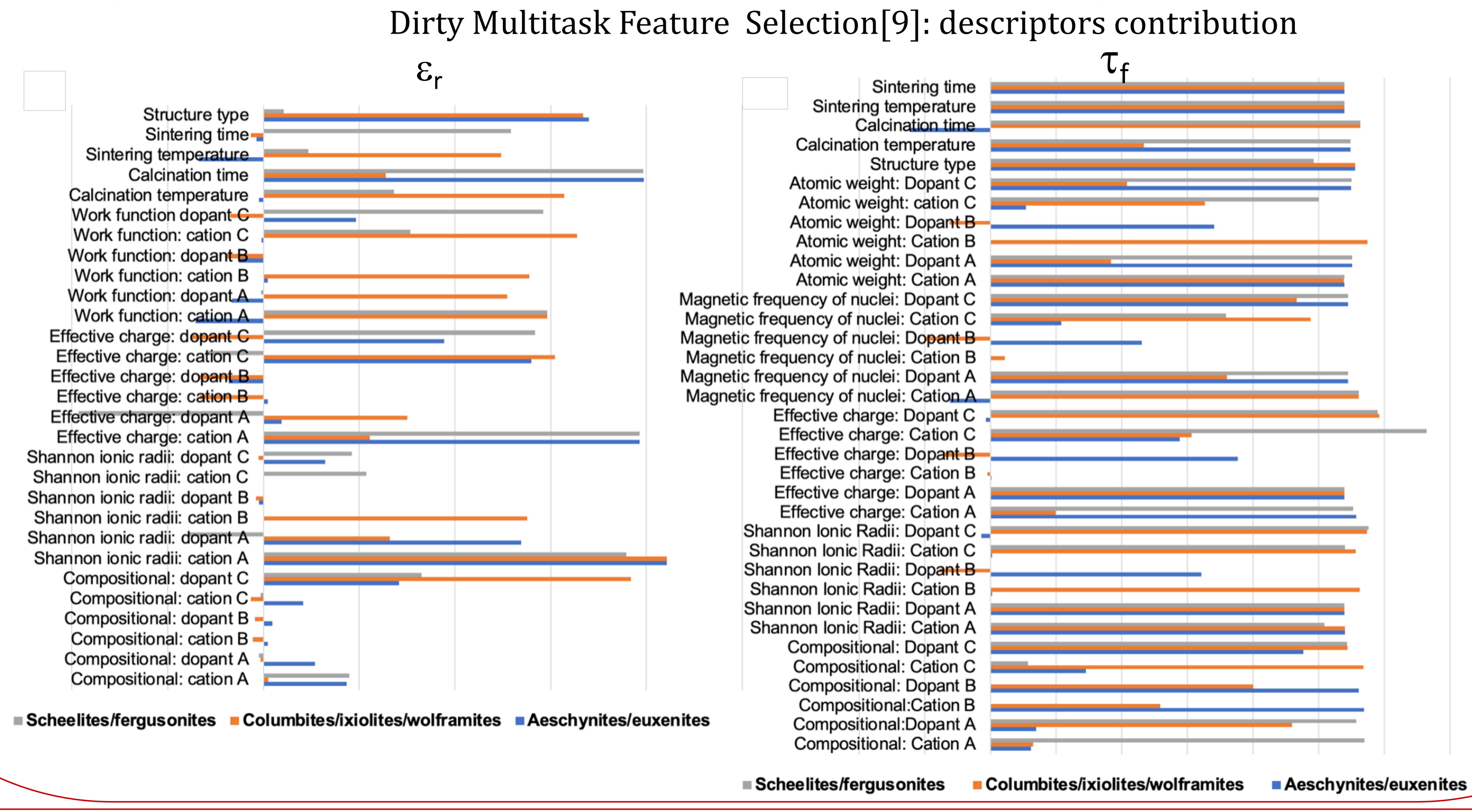


Results of Modeling

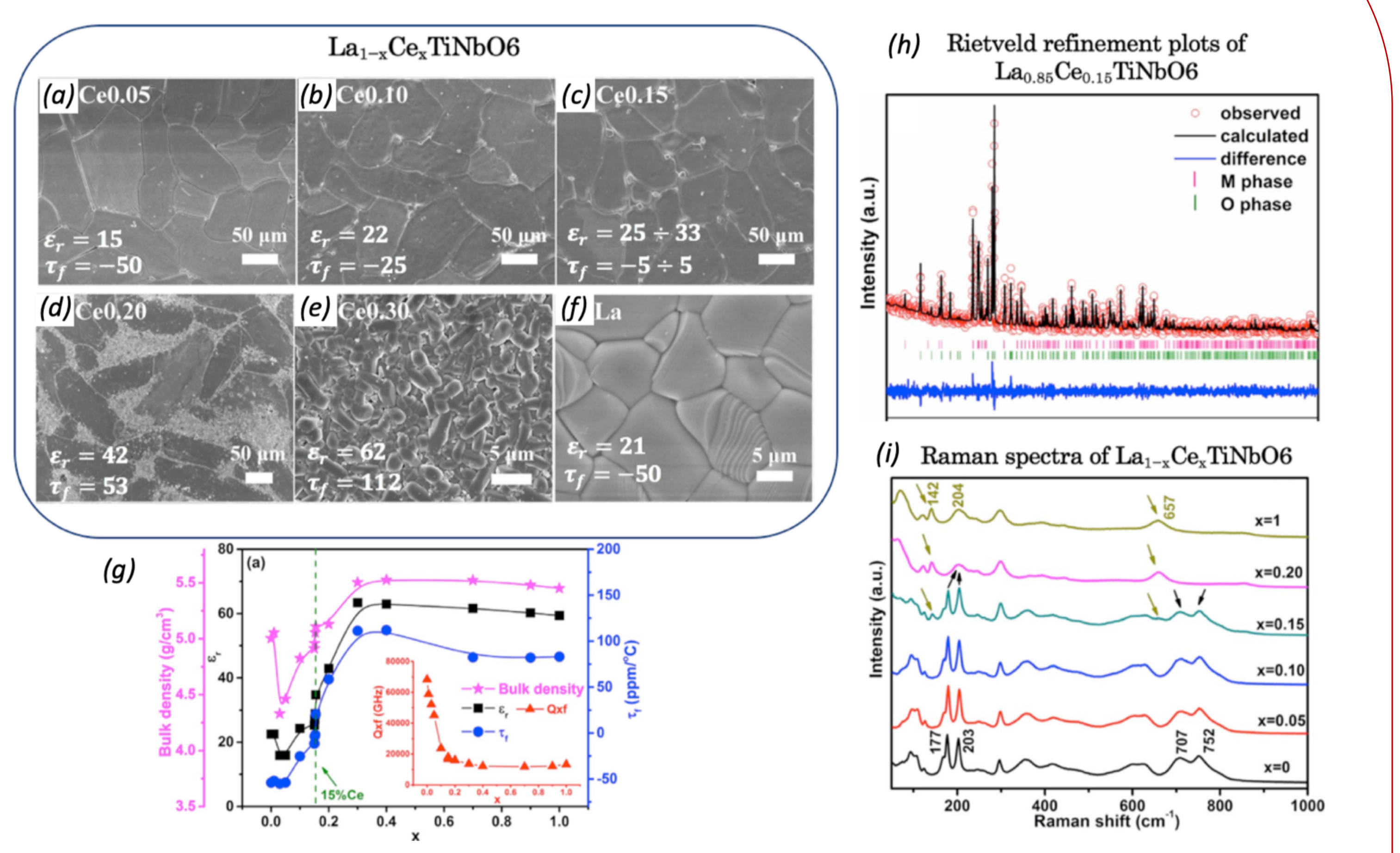
Method: SVM regression [8], five-fold cross-validation
Parameters optimization:
$C = 2^{-5}, 2^{-3}…2^{15}$, ε = 0.0001, 0.001 …10 and γ = 2− 15, 2− 13 …23.



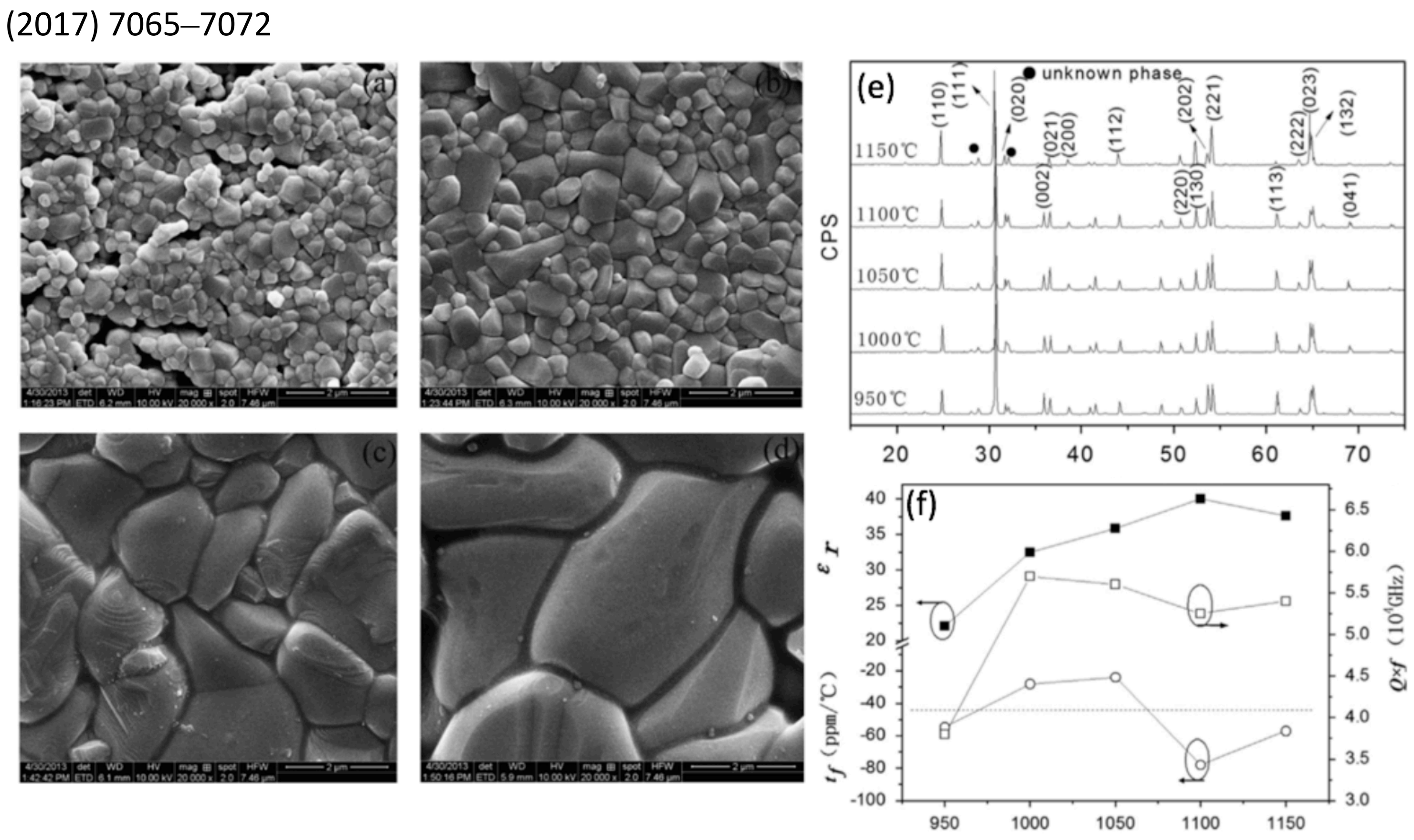
Dirty Multitask Feature Selection[9]: descriptors contribution



Microstructure and Dielectric Characteristics



With permission from J. Zhang, et al Phase structural transition and microwave dielectric properties in isovalently substituted la1-xlnxtinbo6 (ln=ce, sm) ceramics, Ceram. Int. 43 (9) (2017) 7065–7072



With permisiion from: Wu, et al Synthesis, characterization, and microwave dielectric properties of $ZnTiTa_2O_8$ ceramics with ixiolite structure obtained through the aqueous sol–gel process, Ceram. Int. 41 (6) (2015) 7645–7650

References

[1] M. Sebastian (2008) Dielectric materials for wireless communication, Elsevier Science.
[2] M. T. Sebastian, R. Ubic, H. Jantunen (2015). Low-loss dielectric ceramic materials and their properties, *International Materials Reviews, 60* (7), 392–412.
[3] D. Scott, P. Coveney, J. Kilner, J. Rossiny, N. N. Alford (2007). Prediction of the functional properties of ceramic materials from composition using artificial neural networks, *Journal of the European Ceramic Society, 27* (16), 4425 – 4435.
[4] D. J. Scott, S. Manos, P. V. Coveney (2008). Design of electroceramic materials using artificial neural networks and multiobjective evolutionary algorithms, *Journal of Chemical Information and Modeling, 48* (2), 262–273.
[5] A. R. Overy, A. B. Cairns, M. J. Cliffe, A. Simonov, M. G. Tucker, A. L. Goodwin (2016). Design of crystal-like aperiodic solids with selective disorder–phonon coupling, *Nature Communications,* 7, 10445.
[6] W. F. Reinhart, A. W. Long, M. P. Howard, A. L. Ferguson, A. Z. Panagiotopoulos (2017). Machine learning for autonomous crystal structure identification, *Soft Matter 13* (27), 4733–4745.
[7] N. Kireeva and Vitaly P. Solov'ev Machine learning analysis of microwave dielectric properties for seven structure types: The role of the processing and composition . *Journal of Physics and Chemistry of Solids 156 (2021) 110178*
[8] C.-C. Chang, C.-J. Lin, Libsvm : a library for support vector machines, LIBSVM : a library for support vector machines Software, available at: http://www.csie.ntu. edu.tw/cjlin/libsvm.
[9] D. Hernandez-Lobato, A probabilistic model for dirty multi-task feature selection, Proc. Int. Conf. Mach. Learn. (2015) 1073–1082.

Acknowledgments

Authors acknowledge Russian Foundation for Basic Research (Project No. 15-29- 09075) for the support. NK thanks Vladislav S. Pervov for fruitful discussions of this work, Denis Ostroumov, Alexander Petrov and Alexei Averin for their help at the beginning of this study.