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Machine learning to determine the fitting parameters of ferroelectric-dielectric nanocomposites dielectric response

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One of the problems of analyzing experimental electrophysical dependences is determining the parameters of the theoretical model that best reproduces the form of measured dielectric response of ferroelectric-dielectric nanocomposites. For complex nonlinear models, such a problem may have several close solutions, be sensitive to the initial approximation, and require significant computational costs. We investigated the possibility of using machine learning for automated determination of the parameters of a physical model intended for forming an experimental state of the ferroelectric-dielectric nanocomposites. The study of ferroelectric-dielectric nanocomposites was conducted based on the Effective Medium Approximation (EMA) [1] and Heywang models [2]. For each model, a set of curves was formed when varying its physical parameters in given regions. Thus, each curve corresponds to a known set of parameters, which allowed us to form a training sample for the regression problem.

Typically, EMA considers a quadratic equation for the effective permittivity of a binary mixture:

$(1-)\frac{(^{*}_{eff}-^{*}_{b})}{(1-n_a)^{*}_{eff}+n_a{}^{*}_{b}}+\frac{(^{*}_{eff}-^{*}_{a})}{(1-n_a)^{*}_{eff}+n_a{}^{*}_{a}}=0$ (1)

here $^{*}_{a}, ^{*}_{b}$ are the relative complex permittivities of components “a” and “b” respectively, and $1-$ are the relative volume fractions of components “a” and “b” respectively, and n_a is the depolarization field factor for the inclusion of type “a”.

Following Heywang model, the expected Arrhenius-type and/or the Mott-type temperature dependences (as well as a general stretched-exponential law) for the effective conductivity of the nanopowders could be modified by introduction of the effective dielectric permittivity. Thus, we use the following fitting function for effective conductivity:

$_{e}ff(T,)=^{0}_{A}()exp[-(\frac{E_A}{(k_B T_{eff}(T))}]$. (2)

Here E_A is an activation energy of the space charges in the cores/shells (A = C or S). The positive fitting parameter varies in the range $0<1$ for a general stretched-exponential law, which includes the Mott law with $=1/4$ and the Arrhenius law with $=1$. Varying one can simulate a possible crossover from the Arrhenius-type dependence to the Mott-type dependence of the effective conductivity.

The analysis shows that it is most appropriate to use machine learning not for direct approximation of the experimental curve by an arbitrary function, but for identification of parameters of a predetermined physical model. In this case, the result of the algorithm remains physically interpretable, and its correctness can be independently verified by restoring the original dependence. The proposed approach allows us to move from sequential numerical fitting of each experimental curve to automated determination of the physical parameters of the ferroelectric-dielectric nanocomposites and can be used for big data analysis.

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References

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