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Model of effective permittivity for dense ferroelectric nanocomposites

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Existing theoretical models of ferroelectric nanocomposites use the effective medium approximation to describe their dielectric and conductive properties. The most common effective medium models (Landau linear mixture approximation, Maxwell-Garnett model, Bruggeman model, etc.) may be invalid for dense nanocomposites when the volume fraction of ferroelectric inclusions exceeds 20-30%. We have proposed several modifications, such as averaging over particle size, finite conductance of the screening shell, and the dipole-dipole cross-interaction effects between the electric polarization (i.e., their electric dipoles) of different ferroelectric nanoparticles separated by shells and a matrix.
The Lichtenecker-Rotter model, which is free from the volume fraction limitations, was used to estimate the effective dielectric constant ϵ_{eff} of the nanocomposite without taking into account the effects of cross-interaction. However, the presence of small particles (size 30 nm or less) should be taken into account, as dipole-dipole cross-interactions can lead to the formation of polar clusters, where the ferroelectric dipoles of single-domain nanoparticles are strongly correlated, and the correlations determine the effective dielectric response of the composite.
The presence for larger submicron particles (size 300 nm or more), which usually split into ferroelectric domains, the cross-interaction effects can lead to correlated motion of ferroelectric domain walls in neighboring nanoparticles, which, in turn, make a significant contribution to the temperature and frequency behavior of the dielectric response of the composite.
The dependence on $\epsilon_P(T, \theta, \omega)$ of the frequency ω and the temperature of the local transition θ of nanoparticles and their polar clusters in a ferroelectric polymer nanocomposite was analyzed taking into account the dipole-dipole cross-interactions. As a result, the equation for θ. was obtained. This equation was successfully applied to calculate the dielectric constant of dense PVDF nanocomposites with 20-30 vol.% of barium titanate nanoparticles. The obtained results can be used for the prediction and development of the flexible and cheap nanocomposite with superior polar and dielectric properties for usage in non-volatile memory cells, energy-saving elements, modulators and sensors.

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Primary authors: BEREZNYKOV, Oleksii; Prof. MOROZOVSKA, Anna (Institute of Physics, NAS of Ukraine); Dr PYLYPCHUK, Oleksandr (Institute of Physics, NAS of Ukraine); Mr STETSENKO, Denis (Institute of Physics, NAS of Ukraine); Dr IVANCHENKO, Serhii (Institute for Problems of Materials Science, NAS of Ukraine)

Presenter: BEREZNYKOV, Oleksii

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