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Computational studies of ferroelectric composites and thin films containing polyvinylidene fluoride (PVDF) and graphene/graphene oxide

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Computational molecular investigations and experimental studies of the ferroelectric properties of new composite nanomaterials based on polymer ferroelectrics and graphene/graphene oxide are presented. Main results of the computational molecular modeling of various nanostructures and the piezoelectric properties of the composites from polyvinylidene fluoride (PVDF)/poly(vinylidene fluoride-trifluoroethylene) (P(VDF-TrFE)) films and graphene/graphene oxide (G/GO) were reviewed and analyzed in comparison with the experimental data at the nanoscale, particularly with atomic force and piezo-response force microscopy (AFM/PFM) data. The performed computational molecular modeling of the graphene/graphene oxide (G/GO) and PVDF ferroelectric polymer composite nanostructures were studied by the different methods using HyperChem tool: molecular mechanics (MM) methods (BIO CHARM), quantum mechanical (QM) calculations based on density functional theory and semi-empirical PM3 method. Experimentally the switching behavior, piezoelectric response, dielectric permittivity and mechanical properties of the films were investigated and found to depend on the presence of G/GO concentration variation. Experimental results qualitatively correlate with those obtained in the calculations. Particularly, computed data of the piezoelectric coefficients d33 for developed PVDF-G/GO models are in line with observed experimental behavior with concentration changes of GO components. Further development with several multilayered GO nanostructures and inserted PVDF chain and layers, having new curved structures after optimization are considered and discussed. The properties of these investigated nanostructures with the GO content dependence for these composites are analyzed. The results obtained in the reviewed and analyzed present study provide important insights into our understanding of the mechanisms of piezoelectricity in such new nanocomposites give us new prospective for further creation, development and applications of novel ferroelectric polymer–graphene/graphene oxide nanocomposites as multifunctional nanomaterials.

Recent Publications

1. Bystrov V S, Bdikin I K, Silibin V, Karpinsky D, Kopyl S, Goncalves G, Sapronova A V, Kuznetsova T and Bystrova V V (2017) Graphene/graphene oxide and polyvinylidene fluoride polymer ferroelectric composites for multifunctional applications. Ferroelectrics 509(1):124-142.
2. Paramonova E V, Filippov S V, Gevorkyan V E, Avakyan L A, Meng X J, Tian B B, Wang J L and Bystrov V S (2017) Polarization switching in ultrathin polyvinylidene fluoride homopolymer ferroelectric films. Ferroelectrics 509(1):143–157.
3. Bystrov V S, Paramonova E V, Bdikin I K, et al. (2013) Molecular modelling of the piezoelectric effect in the ferroelectric polymer poly(vinylidene fluoride) (PVDF). J. Mol. Mod. 19(9):3591-3602.
4. Bystrov V S (2014) Molecular modeling and molecular dynamic simulation of the polarization switching phenomena in the ferroelectric polymers PVDF at the nanoscale. Physica B: Condensed Matter 432:21-25.

Biography

Vladimir S Bystrov has completed PhD, Dr. Habil.Phys. Dr.Sci. Phys. & Math. from Russian Academy of Sciences. Since 1993, he has his expertise in various fields of computational molecular modeling, computational exploration and computer simulation of nonlinear multifunctional nanomaterials and different organic & bio-molecular nano-structures such as: bioferroelectric & polymer PVDF/PVDF-TrFE thin ferroelectric films, graphene/oxide graphene and related polar composite nanomaterials; amino acids (glycine, etc.), peptides nanotubes, thymine & DNA; hydroxyapatite (HAP) & nanoparticles, etc. Computational studies of nanostructures were made using the molecular mechanics, quantum-chemical calculations (ab initio, DFT, semi-empirical methods), molecular dynamics (MD) on the base of various software (HyperChem, AIMPRO, VASP, etc.) and clusters in Russia IMPB & KIAM, Linux cluster in University of Aveiro, Portugal. He is a Head of the Group for Computer Modelling of Nanostructures and Biosystems of IMPB-KIAM RAS, Pushchino.

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