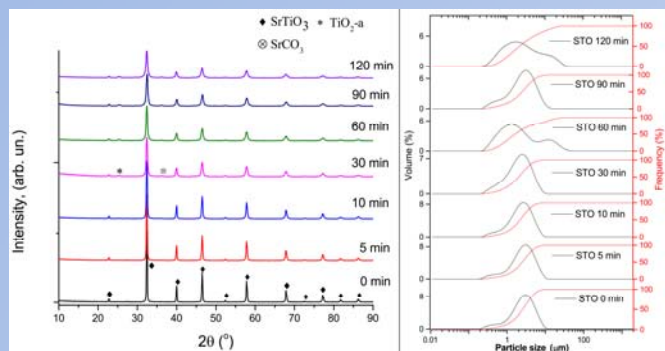


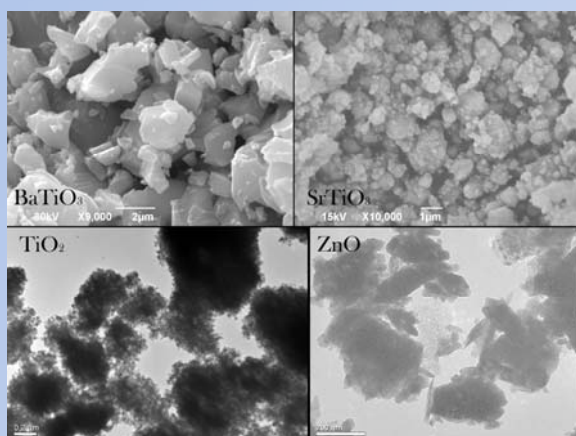
Influence of mechanical activation on mechanical properties of PVDF-nanoparticle composites

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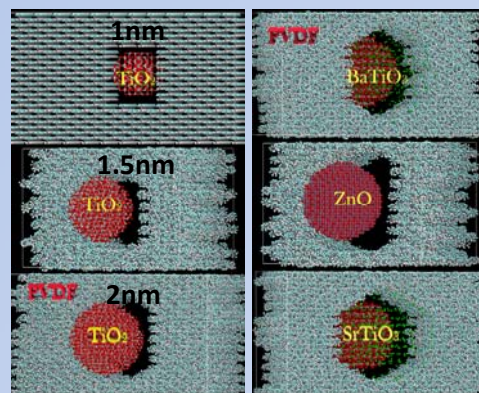
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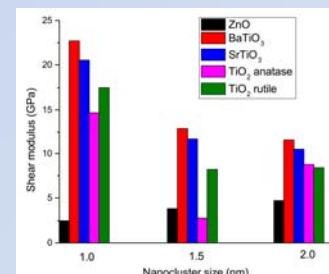
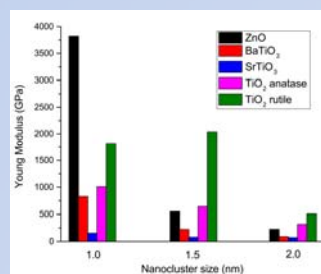
Mechanical activation leads to the creation of new surfaces and decrease in particle size of the initial powder particles, which affects the crystallization of PVDF matrix. In addition, prolonged mechanical activation leads to agglomeration of nanoparticles agglomerates of different sizes.



Microstructural changes due to mechanical activation in ZnO, BaTiO₃, SrTiO₃ and TiO₂ powders were investigated using electron microscopy (TEM and SEM), x-ray diffraction (XRD) and particle size analysis (PSA). These were correlated with molecular simulations of PVDF-nanocluster composites with different oxide nanocluster sizes (1, 1.5 and 2 nm)



Each system was simulated using a periodic system of metal oxide nanocrystal inside β -PVDF matrix. β -PVDF was chosen for its superior properties over α - and γ - phases. Geometry of each system was optimized prior to the calculation of mechanical properties using GULP v4.3 software package.



Molecular simulations show that, in general, mechanical properties (Young modulus as an indication of elasticity, Shear modulus as an indication of hardness) for all systems improve with decrease in nanocluster size. This suggests that mechanical activation of fillers in PVDF-metal oxide nanoparticle composites should have a positive effect on the mechanical properties of composite systems.

This suggests mechanical activation as an easy and inexpensive method of improving mechanical properties of polymer-nanocrystal composite materials.