

ST-P001

Synthesis and Characterization of Lead Zirconium Titanate Nanofibers by Electrospinning

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Lead zirconium titanate (PZT) is usually used as bulk and thin films. Due to high flexibility and piezoelectric, ferroelectric and pyroelectric properties, PZT fiber has attracted in a variety of fields such as sensor devices, non-electromechanical systems and non-volatile ferroelectric memory devices. And PZT fiber can be numerously synthesized and almost with the diameter of PZT fiber thicker than 10 μ m. However, the electrospinning method is cost effective and convenient. PZT obtained by electrospinning method has the diameter from sub-micro to nanometer. In this paper, the PZT/PVP nanofibers were synthesized with three precursors, lead nitrate, zirconium ethoxide and titanium isopropoxide. And the PZT nanofibers were fabricated after removal of PVP by annealing process at various temperature. The obtained PZT nanofibers were characterized by means of X-ray photoelectron spectroscopy (XPS) for chemical properties, X-ray diffraction (XRD) for crystallinity and phase, scanning electron microscopy (SEM) for morphologies. The diameter of PZT nanofibers were measured with SEM. From the SEM images, we confirmed that diameter of PZT nanofibers was hundreds of nanometers and decreased with increasing the annealing temperature. When the annealing temperature increased, the crystallinity of PZT nanofibers changed from pyrochlore to perovskite structure.

Keywords: PZT, electrospinning, XPS

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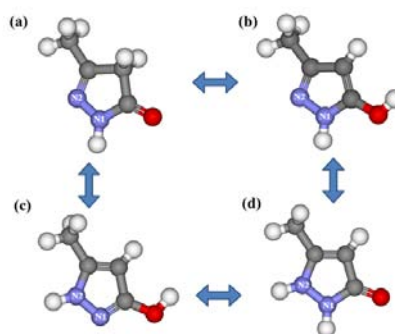
The Adsorption of the 3-methyl 5-pyrazolone on the Ge(100) Surface

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The most stable adsorption structures and energies of four tautomerized forms (keto-1, enol-1, keto-2, and enol-2) of 3-methyl 5-pyrazolone (MP) adsorbed on Ge(100) surfaces have been investigated by Density Functional Theory (DFT) calculation method. Among its four tautomerized forms, we confirmed three tautomerized forms except keto-1 form show the stable adsorption structures when they adsorbed on the Ge(100)-2 \times 1 surface as we calculate the respective stable adsorption structures, activation barrier, transition state energy, and reaction pathways. Moreover, among three possible adsorption structures, we acquired that enol-2 form has most stable adsorption structure with O-H dissociated N-H dissociation bonding structure.

Keywords: Tautomerism, 3-methyl 5-pyrazolone, Density Functional Theory (DFT) Calculation, Ge(100) surface



Scheme 1. The different four structure of 3-methyl 5-pyrazolone's tautomerism. (a) Keto-1 form (b) Enol-1 form (c) Enol-2 form (d) Keto-2 form. The gray, blue, red and white colored balls indicate carbon (C), nitrogen (N), oxygen (O), and hydrogen (H), respectively.