Enhanced electroactive β-phase formation in electrospun poly (vinylidene fluoride-co-hexafluoropropylene) nanowires with gold nanoparticles

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As a representative piezoelectric polymer, poly (vinylidene fluoride-co-hexafluoropropylene) (PVDF-HFP) has been widely used in sensors transducers and actuators. In this paper, gold nanoparticles (AuNPs) are prepared and doped into the PVDF-HFP solution to enhance the piezoelectric property of electrospun PVDF-HFP nanowires. The results indicate that proper amounts of AuNPs within the nanowires can improve the piezoelectric phase in PVDF-HFP. Then, a nanogenerator was prepared using the PVDF-HFP/Au nanowires to verify the increase in piezoelectric performance. Experimental results show that compared with PVDF-HFP nanogenerator without AuNPs doping, the output voltage is increased by about two times, while the output current is doubled for the PVDF-HFP/Au nanogenerator. Furthermore, systematic molecular dynamics (MD) simulations are conducted to elucidate the physical mechanism of AuNPs enhanced β-phase formation in PVDF-HFP. Our results show that the adsorption and electrostatic interaction between the AuNPs and the PVDF chains promote the electroactive β-phase formation, and also significantly increase the tension and poling effect during electrospinning process, which is the origin of the enhanced electroactive phase formation in electrospun PVDF-HFP nanowires.

PVDF-HFP nanowires, β-phase, Gold nanoparticles

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1. Introduction

Polymers with high piezoelectric responses have great application potentials in health monitoring systems, human/machine interaction, soft robot, and so on [1]. As an important class of piezoelectric polymers, poly (vinylidene fluoride-co-hexafluoropropylene) (PVDF-HFP) can exhibit efficient piezoelectricity and pyroelectricity when polarized under high voltage [2-4]. Furthermore, PVDF-HFP is low cost, lightweight, highly stretchable, and biocompatible, which makes it widely utilized in flexible transducers, actuators, and sensors [5,6]. PVDF-HFP is a semi-crystalline polymer with complex polymorphisms, the piezoelectricity of which is closely associated with its crystalline structures [7]. There are five different polymorphs that exist in PVDF-HFP crystals, i.e., α, β, γ, δ, and ε [8,9]. The α-phase crystal is trans-gauche-trans-gauche (TGTG’) conformation and nonpolar with a monoclinic lattice [10]. Both the β- and γ-phase are orthorhombic. The β-phase presents zigzag all-trans chain (TTTT) conformation [11], and the γ-phase presents T₅G₅T₅G’ chain conformation [12]. The δ-phase is polar analog of the α-phase, and ε-phase is antipolar analog of the γ-phase [13]. Among all the phases of PVDF-HFP, the β-phase exhibits the best piezoelectric properties and has the highest polarization. Therefore, promoting the contents of β-phases is required to achieve better piezoelectric performance.

Generally, PVDF-HFP exhibits the nonpolar α-phase. However, the crystalline phases of PVDF-HFP could be changed under thermal [14], mechanical [15,16], or electric
field poling [17,18]. Thus, different methods have been proposed to promote the α- to β-phase transformation, such as high electric field poling, uniaxial stretching, and addition of nanoparticles. Recently, it has been found an effective strategy to promote β-phase formation and enhance PVDF-HFP piezoelectricity by doping nanomaterials into PVDF-HFP to form polymer nanocomposites. Priya and Jog [19] reported the crystal transformation from the α-phase to β-phase by combining PVDF-HFP and nanoclay. Similar polymorph changes have also been realized in PVDF-HFP nanocomposites doped with silver nanoparticles and single wall carbon nanotubes (SWNTs) [20,21]. The crystal transformations certainly favor the piezoelectricity of PVDF-HFP and enhance its piezoelectric responses and mechanical transduction. Moreover, doping nanomaterials into polymers not only changes the crystalline morphology and the piezoelectric properties, which might also have effects on mechanical and thermal properties of polymers. When saponite was doping into nylon 6, the γ-phase of material was formation, and at the same time the toughness was also improved [22].

In order to analyze the phase transformation of PVDF at molecular scale, not only the experimental investigations but also the numerical studies have been conducted. Satyanarayana et al. [23,24] performed molecular dynamics (MD) simulation on the α to β-phase transformation due to stretching and poling and analyzed the torsion angle distribution of PVDF in melting state. Hong et al. [25] used experiments and MD simulations to investigate the phase transformation of PVDF/TiO₂ nanocomposite film. The results show that between hydrogen atoms in PVDF chains and the oxygen atoms on the surface of titanium dioxide particles exist the electrostatic interaction, which can enhance formation of β-phase in PVDF. Sahihi et al. [26] used all-atom MD simulation to investigate the interfacial interaction in the magnetite reinforced PVDF system, and found that the α to β-phase transformation is due to the hydrogen bond interactions between hydroxyl on the surface of magnetite and the PVDF chains.

All the previous studies show that mechanical stretching, electric poling, and interaction from doped nanoparticles play key roles in the conformation transformation of PVDF polymers. It is known that gold nanoparticle (AuNP) is antibacterial and biocompatible, which makes it a perfect candidate to be used in health monitoring sensors, human/machine interfaces, and soon [27]. While electrospinning is a versatile and variable technique to fabricate polymer nanowires, which inherently utilizes high electric field to stretch charged polymer solutions [28]. Therefore, electrospinning is adopted in this study to fabricate PVDF-HFP nanowires, as shown in Fig. 1. AuNPs (0.5wt.%) are prepared and then doped to the PVDF-HFP solution to promote the β-phase formation in electrospinning process. Later, microstructure of the fabricated nanowires and the AuNPs are characterized by scanning electron microscopy (SEM) and transmission electron microscopy (TEM), respectively. The α and β-phase content are analyzed through Fourier transform infrared (FTIR) spectroscopy, X-ray diffraction (XRD), and differential scanning calorimetry (DSC). Then, a nanogenerator is prepared using the fabricated PVDF-HFP/
Au nanowires and tested to evaluate its piezoelectric performance. Furthermore, MD simulations are performed to elucidate the mechanism of phase transformation of PVDF-HFP fibers using electrospinning and AuNP doping. Changes in the dipole moment of PVDF-HFP chains and the dihedral angle are analyzed and presented.

2. Experiments

2.1 Materials preparation

Firstly, the AuNPs with a diameter of 5 nm were prepared based on the method proposed in Ref. [29]. Then, the AuNPs were dispersed in PVDF-HFP solution uniformly, and the electrospinning was used to prepare the nanowires. After drying at 80°C for 30 min, the solvent was removed, and the PVDF-HFP/Au nanowires were prepared. The Ag interdigitated electrode was used as the electrode (linewidth is 30 μm, and spacing is 50 μm). The PVDF-HFP/Au nanowires doped with AuNPs were spun at the ends of interdigitated electrodes by direct electrospinning. The electrode was packed two times with diluted n-hexane: Polydimethylsiloxane (PDMS) (1 : 1) and undiluted PDMS. Vacuum treatment of packaged devices eliminates residual bubbles in the electrodes. The electrodes are polarized at 120°C with 9 V μm⁻¹ voltage, and finally the piezoelectric nanogenerator was obtained.

2.2 Microstructure characterization and piezoelectric performance

Figure 2a is the SEM of PVDF-HFP nanowires, and Fig. 2b is the TEM of AuNP. It is seen that PVDF-HFP solution has good spinnability and obtains good fiber structure. The PVDF-HFP nanowires obtained by electrospinning have a smooth surface, uniform thickness, and a diameter of 300 nm. While the AuNPs are about 5 nm. Figure 2c and d are the SEM of PVDF-HFP/Au nanowires and the TEM of PVDF-HFP/Au nanowires, respectively. The diameter of PVDF-HFP/Au nanowires is about 200 nm, which is smaller than undoped nanowires. The PVDF-HFP/Au nanowires were randomly distributed, and the AuNPs dispersed well in the nanowires along the fiber direction. Doped AuNPs would not destroy the nanostructure of PVDF-HFP. Figure 2e is the energy dispersive X-ray spectroscopy (EDX) of PVDF-HFP/Au nanowires. The results showed that the peaks of C, F, O, and Au appeared, indicating that AuNPs were doped successfully in PVDF-HFP.

The FTIR (Fig. 3a and b), XRD (Fig. 3c), and DSC (Fig. 3d) show that the PVDF-HFP/Au nanowires contain both α-phase and β-phase, where the β-phase can be promoted by doping AuNPs. The FTIR in Fig. 3a shows that PVDF-HFP/Au has the typical characteristic peaks of PVDF-HFP in β-phase [30]. In contrast, the α-phase absorption peaks of PVDF-HFP/Au nanowires decreased or disappeared, which means a decrease of α-phase content in PVDF-HFP [31,32]. As shown in Fig. 3b, due to the interaction between AuNPs and PVDF-HFP, the absorption peak moves towards lower wavenumber in PVDF-HFP/Au [33]. Figure 3c illustrates that the PVDF-HFP nanowires exhibit three peaks of diffraction at the angles of 2θ = 18.8°, 20.2°, and 26.6°. From Ref. [34], we know that these peaks correspond to (020), (110), and (021) of α-phase. Hence, such a result indicates that the crystal structure of PVDF-HFP nanowires is mainly α-phase. In the case of PVDF-HFP/Au nanowires, however, the magnitude of such three peaks decreased obviously, while a new peak appears at 2θ = 20.6° that corresponds to the β-phase (110) [35]. At the same time, the intensity of peak at 2θ = 38.2° increases, which is attributed to the β-phase (200) [36]. Due to that the all-trans TTTT conformation of the β-phase is more than the ‘TGTG’ conformation of the α-phase, we get that the melting point of PVDF-HFP with α-phase is lower than that of the case with β-phase. As shown in Fig. 3d, one sees that the melting temperatures of PVDF-HFP and PVDF-HFP/Au are 167°C and 170°C, respectively. This higher shift of melting temperature shows that such materials are indeed regulated from the α-phase transferred into the β-phase, where the main reason is attributed to the strong interaction between the PVDF-HFP chains and the surface of the AuNP [37].

In order to measure the piezoelectric properties of PVDF-HFP/Au, a nanogenerator of PVDF-HFP/Au was prepared. Before the electric measurement, the nanogenerator is po-
larized under a 5 kV mm$^{-1}$ electric field at 110°C for 30 min. The linear motor (LinMot E1100) is connected to a round plastic stick with a diameter of 1.5 cm and is used to periodically drive the nanogenerators. The equipment used to measure the output voltage and current is Low noise pre-amplifiers (SR570, SR560), and PCI-6259 (National Instruments) is used for data collection. In order to realize real-time data acquisition and analysis, a software platform based on LabVIEW is used. Figure 4a and b is the structures of PVDF-HFP/Au nanogenerator. Figure 4c presents the output voltage of PVDF-HFP/Au and PVDF-HFP nanogenerator, and Fig. 4d is the output current of PVDF-HFP/Au and PVDF-HFP nanogenerator. From Fig. 4, it can be seen that the output voltage of PVDF-HFP/Au nanogenerator is up to

Figure 3  a, b The FTIR of PVDF-HFP/Au and PVDF-HFP nanowires; c the XRD of PVDF-HFP/Au and PVDF-HFP nanowires; d the DSC of PVDF-HFP/Au and PVDF-HFP nanowires.

Figure 4  a, b The structures of PVDF-HFP/Au nanogenerator; c the output voltage of PVDF-HFP/Au and PVDF-HFP nanogenerator; d the output current of PVDF-HFP/Au and PVDF-HFP nanogenerator.
11.2 mV, and the output current is up to 0.21 nA. Compared with the undoped PVDF-HFP nanogenerator, the output voltage increases by about two times, while the output current is doubled. The above results show that doping AuNPs can effectively increase the content of β-phase in PVDF-HFP/Au nanowires and enhance the piezoelectrical properties of the nanogenerator.

3. Theoretical modelling

3.1 Molecular design

To elucidate the physical mechanism of the AuNP enhanced β-phase formation in the PVDF-HFP/Au during the electrospinning process, molecules shown in Fig. 5 are designed based on the experiments [7-10]. Figure 5a shows a unit cell of the α-phase PVDF crystalline. Figure 5b is a geometrically optimized α-phase PVDF-HFP chain. Figure 5c shows the unit cell lattice of cubic Au. The spherical AuNP with a diameter of 5 nm is built from the supercell of this unit cell, as shown in Fig. 5d. The obtained AuNP and the α-phase PVDF-HFP chains are assembled into an empty box to investigate the mechanism of enhanced phase transformation due to AuNP.

3.2 Force field

The polymer consistent force field (PCFF) [38,39] was adopted to characterize the MD of PVDF-HFP molecules. The total force field consists of valence and non-bonded terms, i.e.,

\[ E_{\text{total}} = E_{\text{valence}} + E_{\text{non-bonded}}. \]  

The valence term, \( E_{\text{valence}} \), is the sum of the bond, angle, and dihedral angle terms, which can be expressed as

\[ E_{\text{valence}} = E_{\text{bond}} + E_{\text{angle}} + E_{\text{dihedral}}. \]

where

\[ E_{\text{bond}} = K_2(c - r_{0})^{2} + K_3(r - r_{0})^{3} + K_4(r - r_{0})^{4}, \]

\[ E_{\text{angle}} = E_a + E_{bb} + E_{ba}, \]

\[ E_{\text{dihedral}} = E_{d} + E_{mbt} + E_{ebt} + E_{at} + E_{aat} + E_{bb13}. \]

In the valence terms Eqs. (3)-(5), \( K_2, r_0, \) and \( r_{0} \) are the bond coefficients, distance between atoms, and the equilibrium bond distance, respectively. \( E_a, E_{bb}, E_{ba}, E_{mbt}, E_{ebt}, E_{at}, E_{aat}, \) and \( E_{bb13} \) are the angle, bond-bond, bond-angle, dihedral, middle-bond torsion, end-bond-torsion, angle-torsion, angle-angle-torsion, and bond-bond-13 terms, respectively.

The non-bonded term, \( E_{\text{non-bonded}} \), is the sum of the van der Waals (VdW) and electrostatic interaction [40], which can be expressed as

\[ E_{\text{non-bonded}} = E_{\text{VdW}} + E_{\text{electrostatic}}. \]

where the VdW term is given by using the 9-6 Lennard-Jones (LJ) potential as follows:

\[ E_{\text{VdW}} = \epsilon_o \left( \left( \frac{r_0}{r} \right)^9 - 2 \left( \frac{r_0}{r} \right)^6 \right) \quad (r < r_c). \]

Here, \( \epsilon_o, r_0, \) and \( r_c \) are the energy parameter, size parameter, and cut-off radius, respectively. The electrostatic interaction term can be given by

\[ E_{\text{electrostatic}} = \frac{C q_i q_j}{\epsilon_e}, \quad (r < r_c), \]

in which \( C, q_i, q_j, \) and \( \epsilon_e \) represent the energy-conversion parameters.

![Molecular models](image)

Figure 5 Molecular models: a α-phase PVDF crystalline unit cell, b single α-phase PVDF-HFP chain, c unit cell lattice of Au, and d Au nanoparticle.
constant, charge of each atom, and dielectric constant, respectively.

The embedded atom method (EAM) potential [41], the most widely used force field for metals, is chosen for the bond interaction between gold atoms. The total force field of an atom \(i\) is given by

\[
E_i = F_{\alpha} r_i \left( \rho_{\alpha}(r_i) \right) + \frac{1}{2} \sum_{j \neq i} \phi_{\alpha\beta}(r_{ij}),
\]

where \(F_{\alpha}\) is the embedding energy which is a function of atomic electron density \(\rho_{\alpha}\), \(\phi_{\alpha\beta}\) is a pair potential, and \(\alpha\) and \(\beta\) are the element types of atoms \(i\) and \(j\).

For the interaction between AuNPs and the PVDF-HFP chains, the 9-6 LJ potential expressed in Eq. (7) is adopted, where \(\sigma\) and \(\epsilon\) are obtained based on the mixing rules, i.e., \(\sigma = (\sigma_{\text{Au}} + \sigma_{\text{unit}})/2\), and \(\epsilon = \sqrt{\epsilon_{\text{Au}} \epsilon_{\text{unit}}}\), in which \(\sigma_{\text{Au}}\) and \(\epsilon_{\text{Au}}\) are the parameters for Au atoms, and \(\sigma_{\text{unit}}\) and \(\epsilon_{\text{unit}}\) are for the atoms in polymer chains.

3.3 Conformation transition of PVDF-HFP/Au

During the electrospinning process, the PVDF-HFP polymer with AuNPs will be subject to large elongation and experience significant poling due to the high electric field. In the simulation, we calculate the dipole moment \(\mu\) of the polymers and present its variation during the elongation and electric poling process. Moreover, we analyzed the probability distribution of C-C-C-C and C-C-C-F dihedrals in the PVDF chains to demonstrate their phase transformation. According to Ref. [42], the C-C-C-C and C-C-C-F dihedrals are about ±60° and ±180° for the α-phase PVDF. While, for the β-phase PVDF, these dihedrals are about ±180° and ±57°, respectively. Thus, increasing the probability of C-C-C-C dihedrals and/or decreasing the probability of C-C-C-F dihedrals at ±180° can be considered a sign of α to β-phase transformation in PVDF. Likewise, decreasing the probability of C-C-C-C dihedrals at ±60° and/or increasing the probability of C-C-C-F dihedrals at ±57° can be considered a sign of α to β-phase transformation.

4. Numerical results and discussions

In order to verify our numerical simulation scheme and the analysis method for phase transformation based on the dihedral distributions, we firstly investigate phase transformation of the α-phase PVDF crystalline shown in Fig. 5a. Then, we investigate the effect of stretching, electric field poling, and AuNPs doping on the phase transformation in PVDF-HFP chains during electrospinning process. All the simulations are performed with the large-scale atomic/molecular massively parallel simulator (LAMMPS) [43].

4.1 Conformation transition of α-phase PVDF crystalline

In Fig. 6, the simulated crystalline structure of the α-phase PVDF lattice subjected to mechanical stretching and electric field poling are presented. Figure 6a1-d1 shows the top, front, left, and perspective view of the original TGTG’ structure of the α-phase PVDF lattice adopted in the simulation. The rectangular simulation-box is of size 4.96 Å × 9.64 Å × 23.1 Å, which contains 2 polymer chains with 10 monomers in each chain. Figure 6a2-d2 shows top, front, left, and perspective view of the lattice structure after a mechanical stretch with the ratio of 100% is applied in z direction. It is obviously seen that the α-phase PVDF lattice totally transits from the TGTG’ conformation into the zigzag-shaped, TTTT (β-phase) conformation. This result demonstrates the effectiveness of our modelling scheme and numerical methods. In addition, we investigated the effect of electric field poling on the phase transformations of the α-phase PVDF lattice. Figure 6a3-d3 presents the top, front, left, and perspective view of the PVDF lattice structure after...
electric field poling in $y$ direction with $E_y = 1$ V/Å. Compared with the original lattice structure, it is found that the positive H atoms and negative F atoms align in the electric field direction, as obviously shown in Fig. 6c3. This alignment leads to the change in the shape of the backbone of the polymer chain and partial conformation transition from TGTG’ to TTTT.

To quantitatively demonstrate the phase transformations in the $\alpha$-phase PVDF lattice, we present the C-C-C-C and C-C-C-F dihedral distribution, and the overall dipole moment evolution in the mechanical stretching and electric poling process in Figs. 7 and 8, respectively. In Fig. 7a, changes in the C-C-C-C and C-C-C-F dihedral distribution of $\alpha$-phase lattice after stretching axially with a ratio of 100% are presented. Both increasing in the probability of C-C-C-C dihedrals and decreasing in the probability of C-C-C-F dihedrals at $\pm 180^\circ$ occur, which demonstrates the $\alpha$ to $\beta$-phase transformation and the availability of our methods for analyzing conformation transitions. Figure 7b shows the overall dipole moment evolution during mechanical stretching. It is seen that the dipole moment sharply varies as the conformation changes with the applied strain. Changes in the C-C-C-C and C-C-C-F dihedral distribution of $\alpha$-phase lattice after electric field poling in $y$ direction, and the overall dipole moment evolution during electric field poling Fig. 8a and b, respectively. Compared with the changes under stretch, although not that obvious, we can also see the increase in the probability of C-C-C-C dihedrals and decreasing in the probability of C-C-C-F dihedrals at $\pm 180^\circ$ under electric poling. As shown in Fig. 8b, the overall dipole moment almost linearly increases with the externally applied electric field.

4.2 Conformation transition of $\alpha$-phase PVDF-HFP/Au

PVDF-HFP is a copolymer, and we first investigate the effect of HFP blocks on the phase transformation of PVDF. As shown in Fig. 9a, the polymer chain becomes straighter as the axial stretch increases. In this process, the PVDF parts in the copolymer deform more severely and experience conformation transformations, as shown in the enlarged image. Figure 9b illustrates the dihedral distribution of the PVDF-HFP chain before and after stretching. It is seen that probability of the C-C-C-C dihedrals decreases at $\pm 60^\circ$ and the C-C-C-F dihedrals increases at $\pm 180^\circ$, which signs that the $\alpha$ to $\beta$-phase transformation happens. The overall dipole moment of the PVDF-HFP chain during mechanical stretching is presented in Fig. 9. Different from that of the $\alpha$-phase PVDF, the dipole moment of the PVDF-HFP chain (shown in Fig. 9c) has a large component in the axial direction due to the presence of the -CF$_3$ groups in the HFP block part. This dipole moment decreases continuously as the copolymer

![Figure 7](image1.png)  
**Figure 7**  
a Changes in the C-C-C-C and C-C-C-F dihedral distribution of $\alpha$-phase lattice after stretching in $z$ direction with ratio 100%.  
b Overall dipole moment evolution during mechanical stretching.

![Figure 8](image2.png)  
**Figure 8**  
a Changes in the C-C-C-C and C-C-C-F dihedral distribution of $\alpha$-phase lattice after electric field poling in $y$ direction.  
b Overall dipole moment evolution during electric field poling.
chain is stretched axially and becomes straighter.

In Fig. 10, we present the simulation results of a PVDF-HFP chain interacting with a AuNP. Figure 10a shows the variation of the potential energy between the polymer chain and the AuNP. It can be found that three stages exist during the interaction. In the first stage, the long range VdW interaction attracts the PVDF-HFP chain moving toward the AuNP. As the polymer chain approaches near the AuNP, it experiences strong repulsion from the Au atoms at the surface due to interatomic interaction. When it surpasses this energy barrier, the polymer chain was stably adsorbed at the AuNP surface through the electrostatic interaction between the H atoms in the chain and the Au atoms at the surface of the AuNP (see the inset image of Fig. 10a). Figure 10b presents the variation in the potential energy at typical points and the corresponding configuration of the polymer chain and AuNP. In addition, energy minimization was performed to the system, and the most favorable configuration and corresponding potential energy are presented, as shown in the red box of Fig. 10b. This signifies that the AuNP has a strong attractive force on the PVDF-HFP chains.

In Fig. 11a and b, we present the dihedral distribution and the overall dipole moment evolution during the absorption of polymer chain by the AuNP. From the dihedral distribution shown in Fig. 11a, we can see that the probability of C-C-C-C dihedrals at ±180° and the probability of C-C-C-F dihedrals at 60° significantly increase due to the presence of the AuNP. This signifies that the electrostatic interaction from AuNP promotes the β-phase formation of PVDF-HFP polymers. In addition, the strong attraction force acted by the AuNP will enhance the mechanical stretching effect in the electrospinning process, which contributes to the α to β-
phase of PVDF-HFP nanowires as well. Figure 11b shows the overall dipole moment evolution during the absorption process of the polymer chains. Similar to the single chain without AuNP, the overall dipole moment also has a large axial component, and it decreases gradually as the polymer chain is absorbed into the AuNP. Meanwhile, the z-axis component of the dipole moment gradually increases in this process.

5. Conclusions

In this paper, we doped gold-nanoparticle with PVDF-HFP and prepared PVDF-HFP/Au nanowires by electrospinning. The effect of gold-nanoparticle doping on the electroactive β-phase formation in PVDF-HFP was studied by a series of structural characterization and performance evaluation. The results show that with the doping of AuNP, the content of β-phase increases significantly in PVDF-HFP nanowires. The nanogenerator prepared by using the electrospun PVDF-HFP/Au nanowires demonstrates a significant improvement in the piezoelectric performance. Its output voltage reaches up to 11.2 mV, and the output current up to 0.21 nA. Compared with the undoped PVDF-HFP nanogenerator, the output voltage increases by about two times, while the output current is doubled. All the experimental results demonstrate that the piezoelectric property of the electrospun PVDF-HFP nanowires has been significantly improved by doping with gold-nanoparticle. MD simulations have been performed to elucidate the physical mechanism of the α to β-phase transformation in electrospun PVDF-HFP nanowires. From the experimental and numerical simulation results, it can be concluded that: (1) mechanical stretching plays a significant role in the α to β-phase transformation of PVDF-HFP polymers; (2) electric field poling made the H and F atoms align with the field direction, which promotes the α to β-phase transformation indirectly; (3) the AuNP has a strong absorption effect on the polymer chains through the electrostatic interaction between surface Au atoms and the hydrogen atoms in the PVDF chains, which lead to the conformation change in the PVDF-HFP. Moreover, the attraction force on the polymer chains may enhance the stretching effect during electrospinning, which will contribute to more electroactive phase formation.

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金纳米粒子掺杂对聚偏氟乙烯-六氟丙烯纳米线压电性能影响研究

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摘要：聚偏氟乙烯-六氟丙烯（PVDF-HFP）作为一种具有代表性的压电聚合物，已广泛应用于传感器和制动器中。本文制备了金纳米颗粒（AuNP），并将其掺杂到PVDF-HFP溶液中，以增强电纺PVDF-HFP纳米线的压电性能。结果表明，在纳米线中加入适量的AuNP可以改善PVDF-HFP中的压电相。然后，使用PVDF-HFP/Au纳米线制备了纳米发电机，以验证压电性能的提高。实验结果表明，与未掺杂AuNPs的PVDF-HFP纳米发电机相比，PVDF-HFP/Au纳米发电机的输出电压提高了约两倍，输出电流增加了一倍。此外，还进行了系统的分子动力学模拟，以阐明AuNPs增强PVDF-HFP中的压电相形成的原因。结果表明，AuNPs和PVDF链之间的吸附和静电相互作用促进了压电性β相的形成，也显著增加了静电纺丝过程中的张力和极化效应，这是静电纺丝PVDF-HFP纳米线中增强的压电相形成的根源。