Influence of internal structure on properties and morphology of nanofiber textiles

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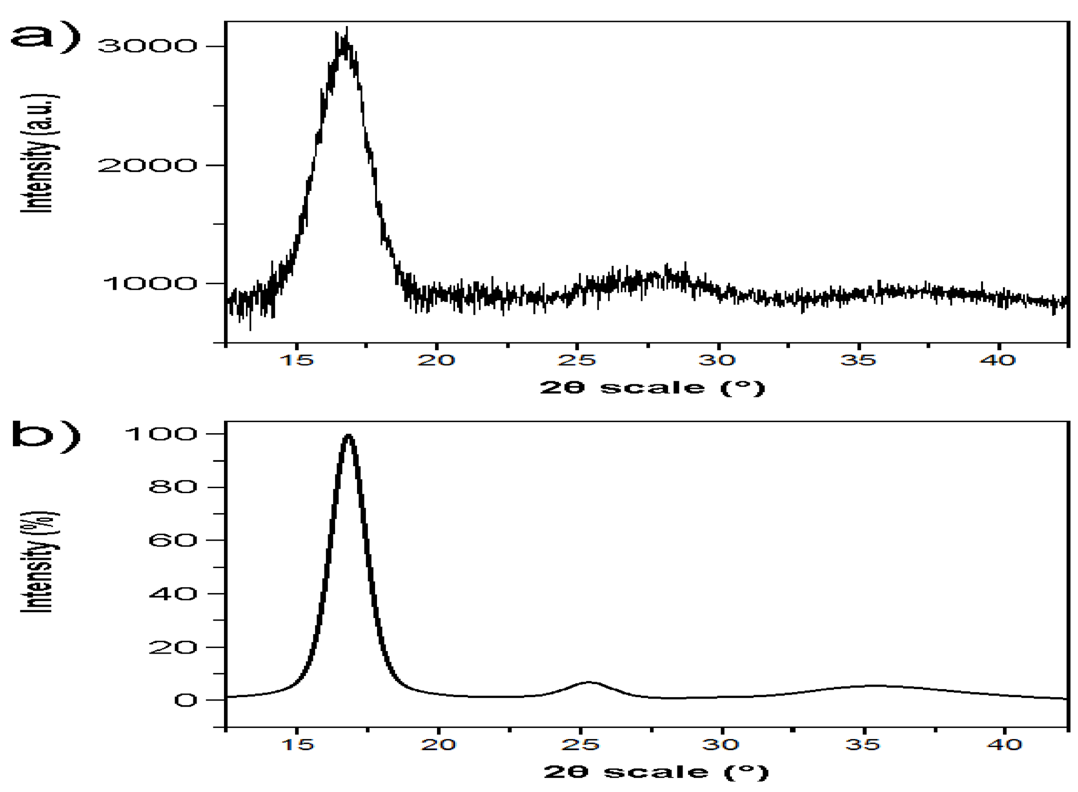
Our previous results showed that crystallization in the strong electric field, especially in case of wire spinning affects the crystal structure and phase composition of nanofibers. In any case the crystal structure is strongly affected by the preferred orientation of crystallites. The texture is typical fiber texture with cylindrical symmetry of distribution function of crystallites orientation. Fiber axis is in polymer chain axis and all the crystallographic planes, which are not parallel with texture axis, are suppressed in XRD powder diagram. This makes the structure and phase analysis very difficult. Anyway the profile analysis of diffraction pattern showed clearly that electrospinning changed the phase composition especially in case of wire spinning.

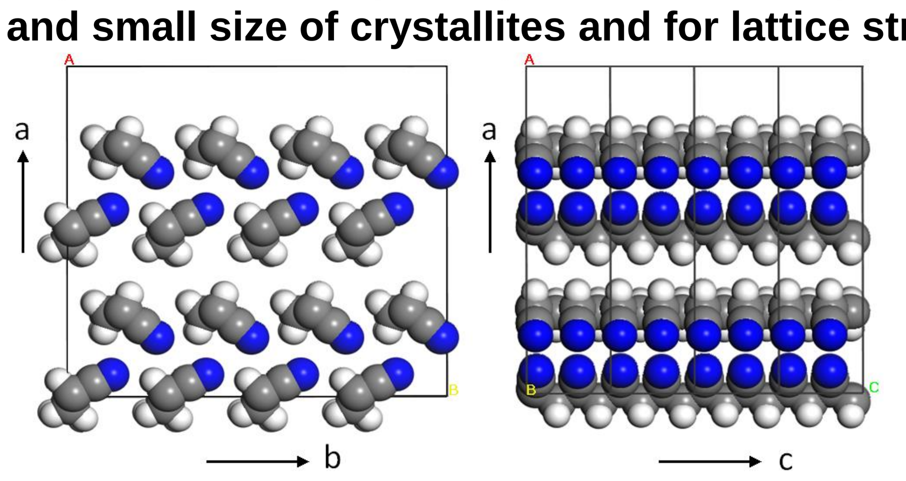
In present work we have found two special cases: PAN and PVDF, where the specific crystal phase in electrospun nanofibers significantly affected the fiber morphology and properties. In both cases electrospinning led to dominant crystal phase, that is characterized by two common features: (1) layered arrangement of chains in crystal structure and (2) charge polarity and electroactivity of these layers, as one can see in the figure 1. Both of these effects lead to the flat shape of crystalline fibers in the form of thin strips, which due to their flexibility and charge distribution roll up into tubes - forming hollow fibers. This work showed that hollow nanofibers can be prepared in a simple way and thus produce a nanofibrous membrane with a higher surface for further chemical modifications, respectively to improve the sound-insulating properties of the membranes.

Polyacrylonitrile



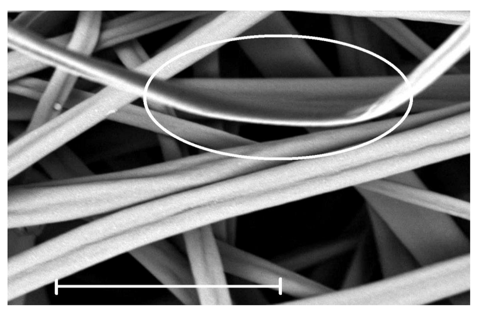
Experimental XRD pattern (radiation CuKα) of electrospun PAN membrane (a)

Simulated diffractogram (b) of optimized model of PAN structure in *Materials Studio* modeling environment by using corrections for preferred orientation and small size of crystallites and for lattice strain.



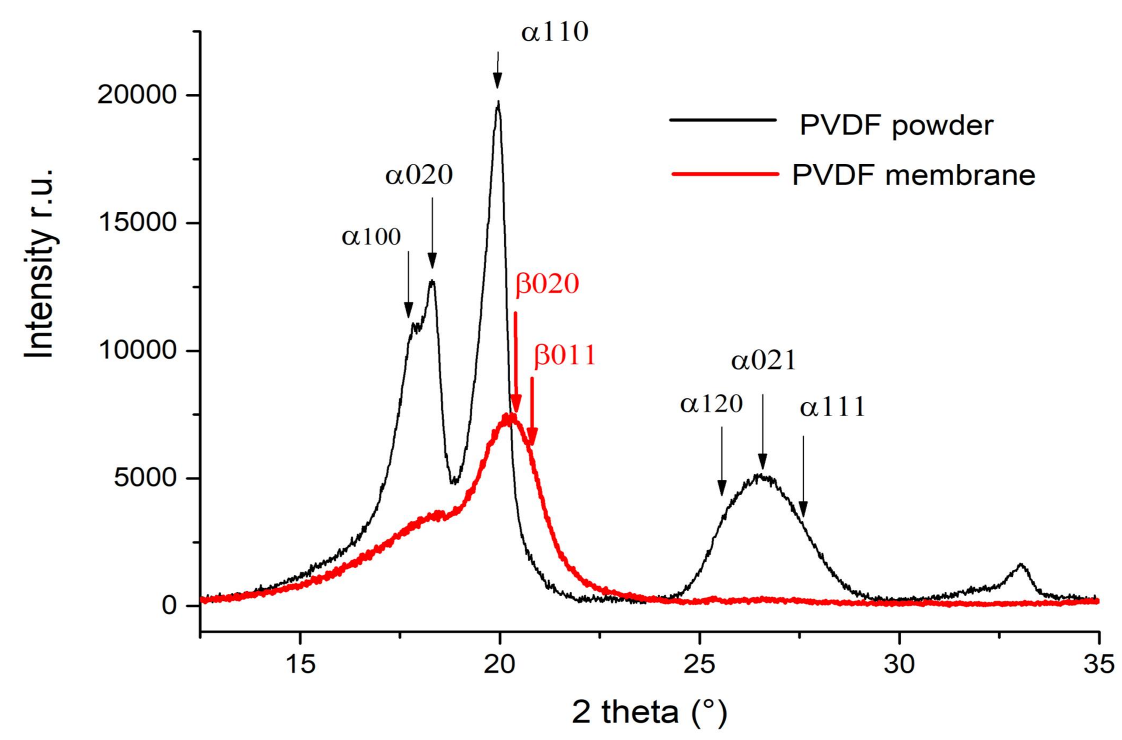
Visualization of PAN nanofiber crystal structure. Unit cell in projection to the *ab* plane (left) and to the *ac* plane (right).

Color legend: C – grey, H – white, N – blue.

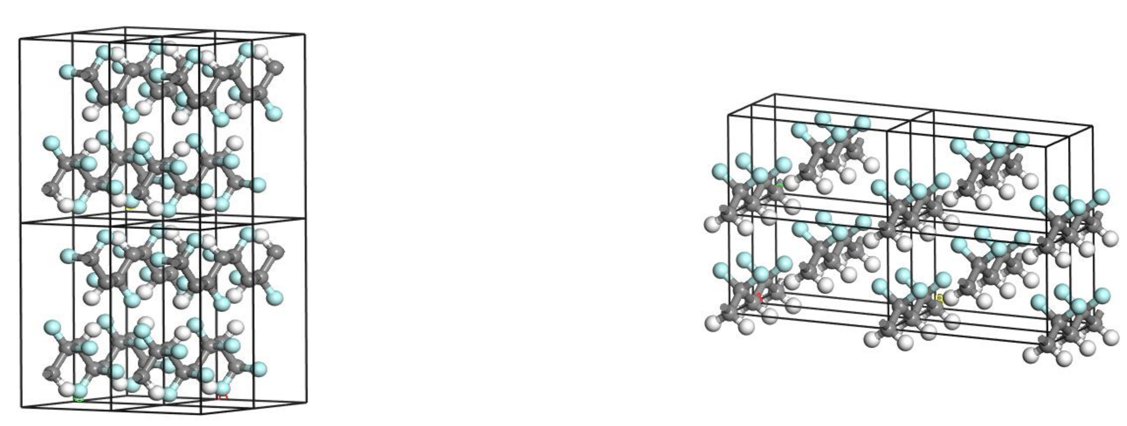


HRSEM image showed the tendency to form strip shaped nanofibers.This strip shaped structure of nanofibers caused longitudinally rolling and due to formation of hollow nanofiber structures.

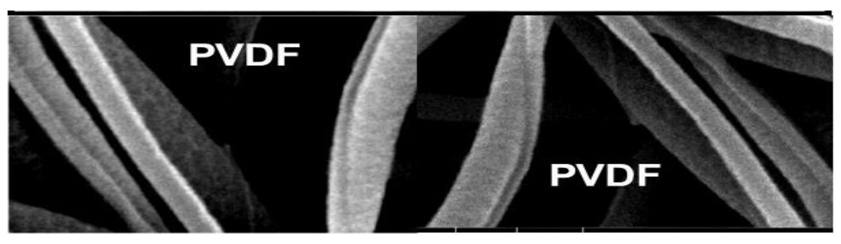
Polyvinylidene fluoride



Comparison of the XRD pattern for PVDF powder and PVDF electrospun nanotextile

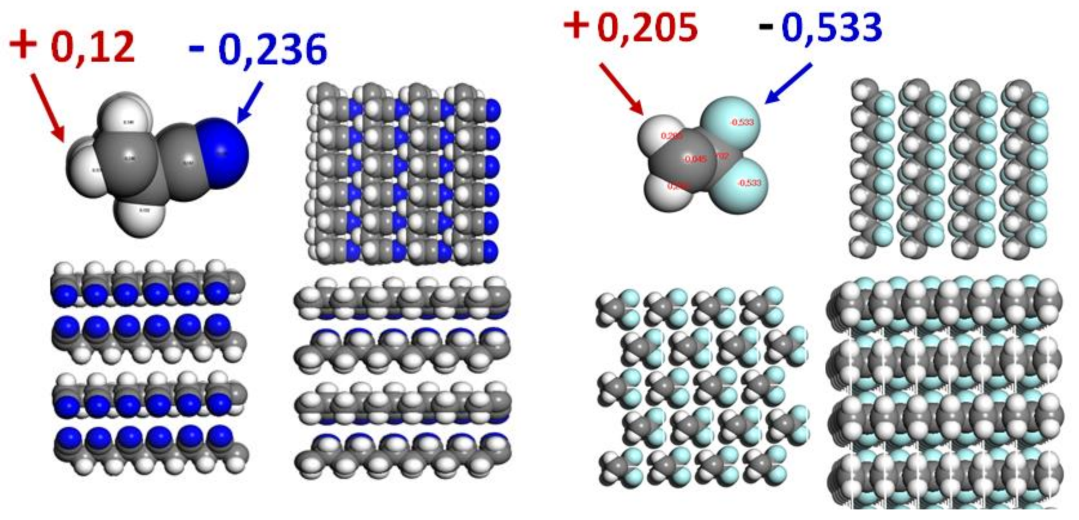


Visualization of crystal structrure for PVDF alpha (left) and beta (right) phase



HRSEM image showed the same tendency to form strip shaped nanofibers as for PAN membranes and also the same formation of hollow fibers

Conclusions



(a) (b)

Illustration of charge distribution in polymer chains for PAN (a) and PVDF (b) in upper left corner (a) and (b). Charges were calculated in Materials Studio modeling environment.

The results of this research show that the internal crystalline structure of polymer chains has a fundamental influence on the properties and morphology of nanofibers prepared by electrospinning. By studying the crystal structure and charges at atoms in the polymer chain, we can relatively accurately predict the properties of the prepared nanotextile.

As two examples, we used polymers PAN and PVDF, which contain dipoles in their structure and their structure is layered. The charge distribution and polymer chain structure is illustrated on the picture on the left side. This structural arrangement lead to the formation of ribbon fibers and subsequently to hollow fibers formation.

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