

Supporting information

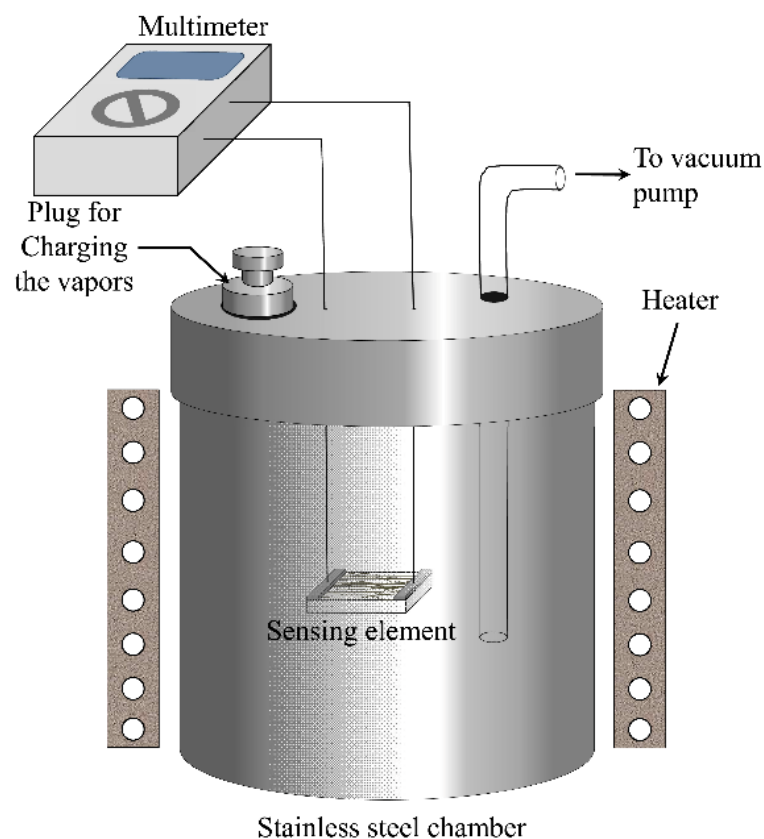


Fig. S1 Schematic of the gas sensing unit

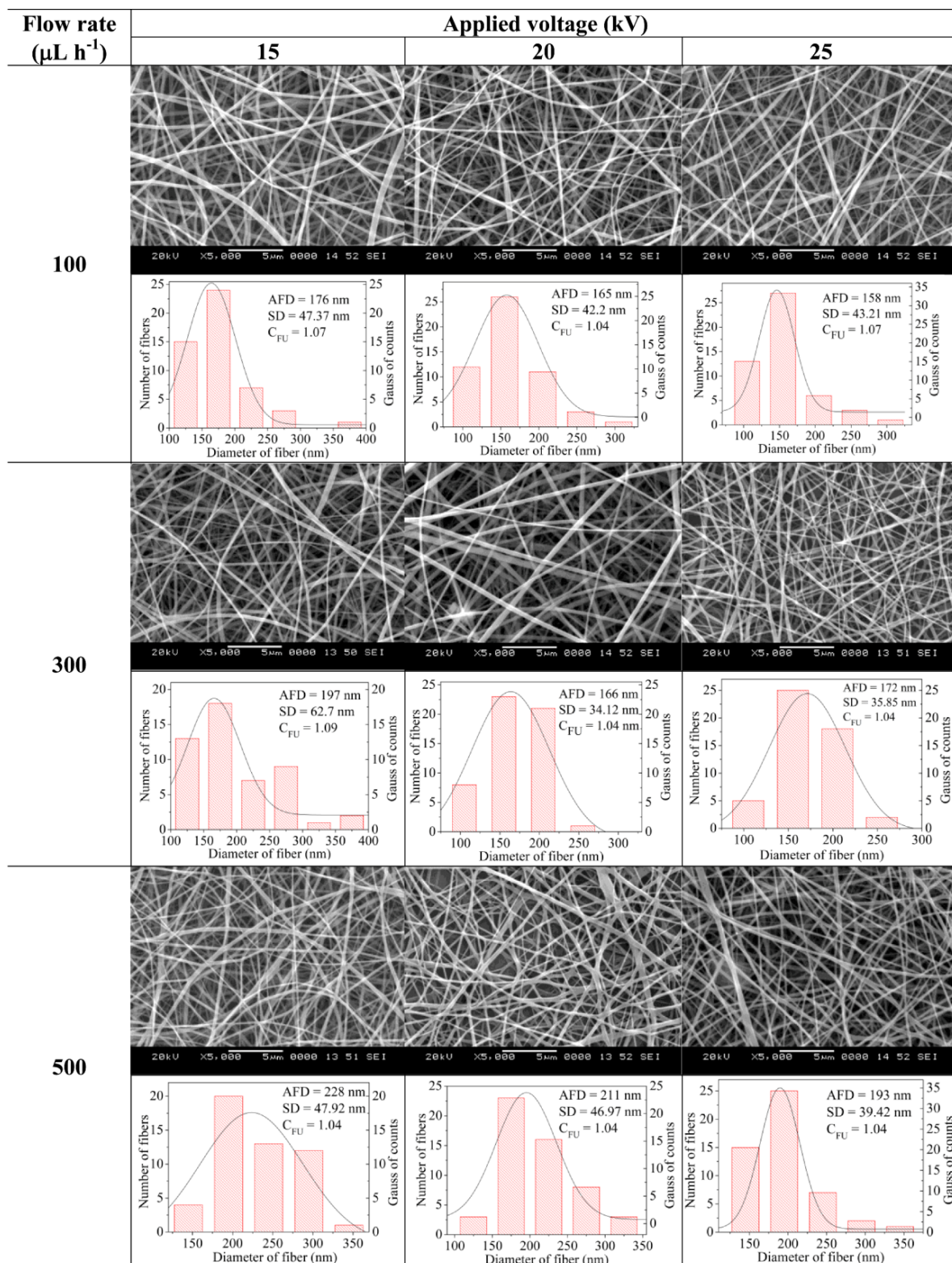


Fig. S2 SEM micrographs and histograms (50 fibres) of electrospun PETox/NATH fibres at different applied voltages (15, 20 and 25 kV) and flow rates (100, 300 and 500 $\mu\text{L.h}^{-1}$). The insets in histogram represent average fibre diameter (AFD), fibre uniformity coefficient (CFU) and standard deviation in fibre diameter (SD).

FTIR spectra of the precursor fibre mats

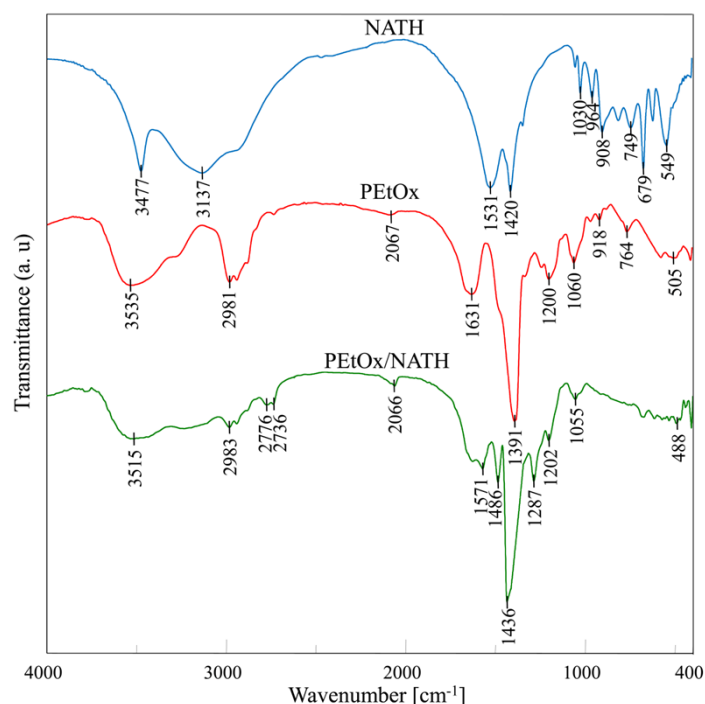


Fig. S3 FTIR spectra of PEtOx, NATH and PEtOx/NATH composite fibres

In all spectra, the peaks $>3400\text{ cm}^{-1}$ are due to OH stretching and the peaks at 2977 and at 2935 cm^{-1} are attributed to the symmetric and asymmetric vibrations of CH_2 , respectively. In the spectrum of NATH, the peaks at 1531 and 1420 cm^{-1} are assigned to the C=O in ionized acetate and C-H deformation in the acetate, respectively. In the spectrum of PEtOx, the peak at 2066 cm^{-1} is attributed to the C=O stretching, the peak at 1633 cm^{-1} is assigned to NH bending, The peaks at $1,391$ and $1,060\text{ cm}^{-1}$ correspond to CH bending and C–O stretching, respectively, and the peak at 1200 cm^{-1} is attributed to the C-N stretching.¹

TG analysis of NiO nanofibers

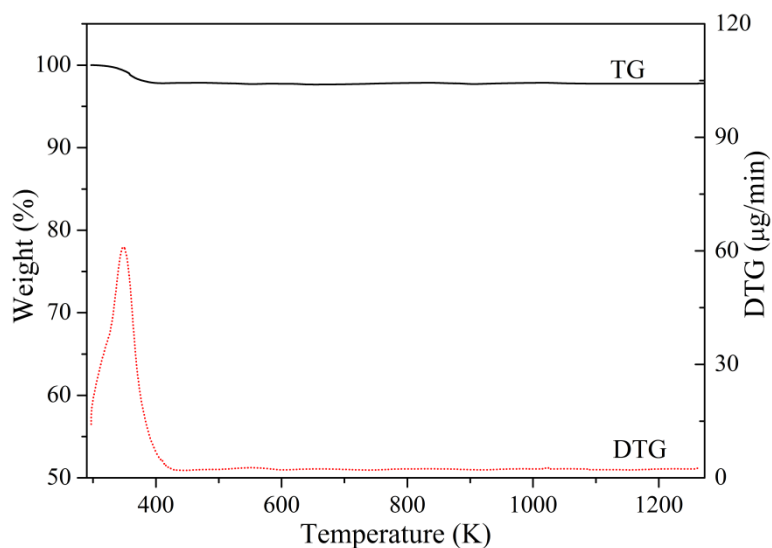


Fig. S4 TG and DTG curves of NiO nanofibers obtained at 673 K .

Determination of Grain size from XRD pattern

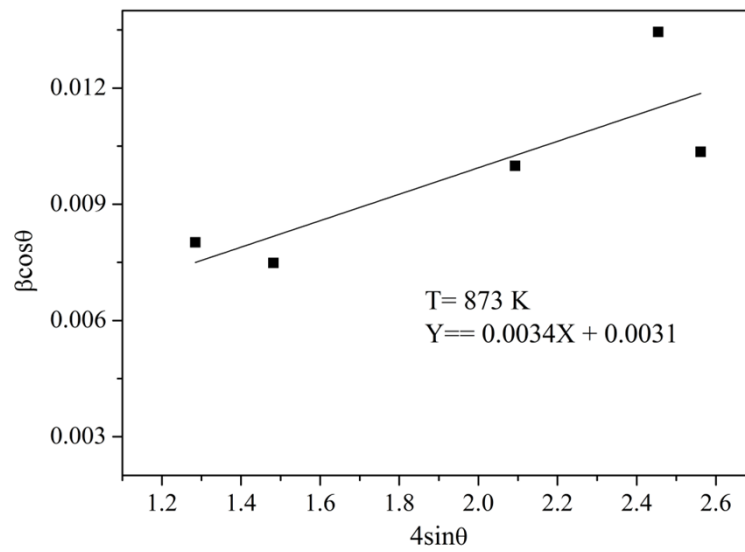


Fig. S5 Williamson-Hall plot for determining crystallite size and lattice strain in NiO nanofibres obtained at 873 K.

Williamson-Hall equation,

$$\beta_{hkl} \cos \theta = \left(\frac{k\lambda}{D} \right) + 4\varepsilon \sin \theta \quad (7)$$

Where, β_{hkl} is the full width at half maximum of the XRD peaks, k is a constant and its value is 0.9, D is the grain size, λ is the wavelength of the x-rays used for the analysis, ε is the induced strain and θ is the Bragg angle. The grain size was calculated from the 'y' intercept of the linear fit of the plot of $\beta\cos\theta$ vs. $4\sin\theta$ (**Fig. S5**).

Grain growth

Arrhenius equation:

$$D = A \exp\left(\frac{-E_a}{RT}\right) \quad (8)$$

Where, D is the average grain size, A is the pre-exponential factor, E_a is the activation energy for atomic/ionic diffusion around the grain boundary, R is the gas constant, and T is temperature in Kelvin.²

Considering E_a as 10.94 kJ mol⁻¹ (ref. 3) and R as 8.314 J K⁻¹ mol⁻¹, the value of A was calculated for the grain size corresponding to the calcination temperature of 673 K. The value of A is 136.37 nm K⁻¹, which was used for the calculation of grain sizes of the fibres obtained

at other temperatures also and the results are presented in **Table 1**.

XPS analysis

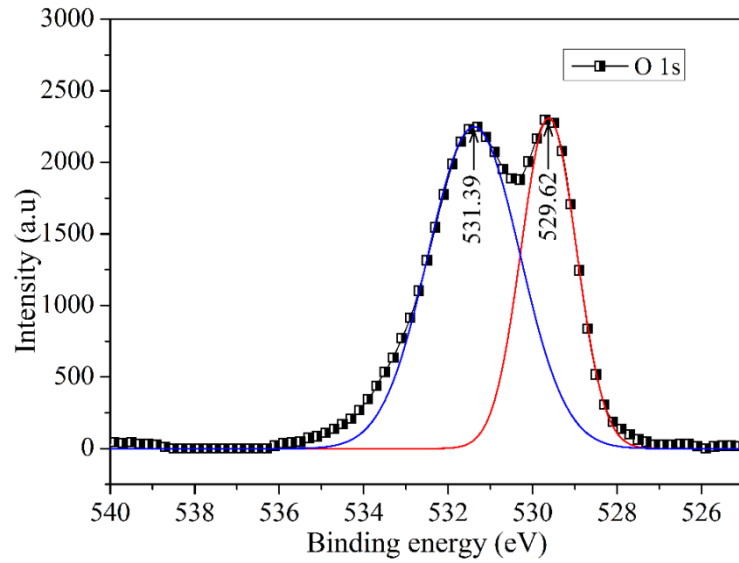


Fig. S6 XP spectrum of oxygen (O-1s)

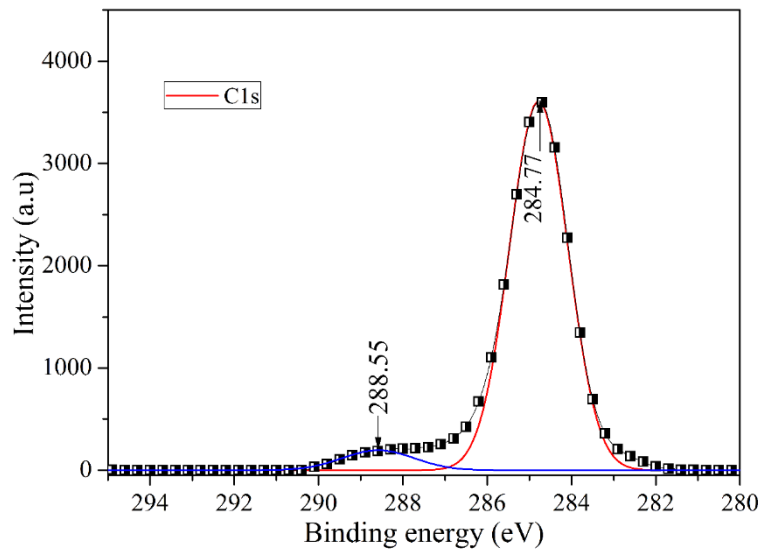


Fig S7 XP spectrum of carbon (C-1s)

Determination of band gap energy and Urbach energy

To determine the band gap energy from the optical spectra, the following relation is used;⁴

$$(\alpha h\nu)^2 \propto (h\nu - E_g) \quad (9)$$

Where, α is the absorption coefficient, $h\nu$ is the photon energy, E_g is the band gap, and n is either 1/2 for an indirect transition or 2 for a direct transition. The intercept of the linear region of the plot $(\alpha h\nu)^2$ vs. $h\nu$ (**Fig. 11b**) with x-axis determines the band gap energy.

Urbach energy is calculated by taking the inverse of the slope of the linear region in the plot of $\ln(\alpha)$ vs. $h\nu$ (**Fig. 11c**).⁵ Urbach energy of the NiO nanofibres obtained at different calcination temperatures are shown in **Table 3**.

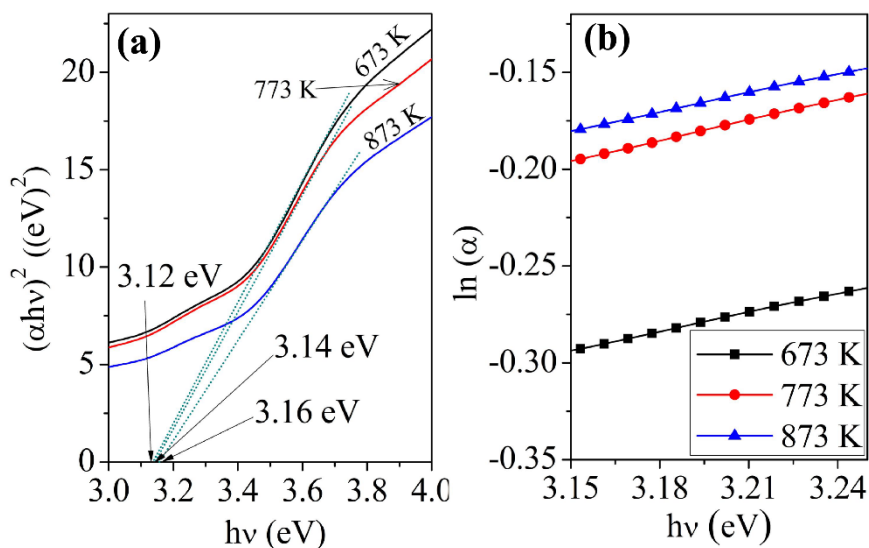


Fig. S8 (a) Determination of band gap from UV spectra (c) Calculation of Urbach energy of NiO nanofibres.

References

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