Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A

Energy efficient role of Ni/NiO in PdNi nano catalyst used in alkaline DEFC

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XRD analysis for calculation of Lattice parameters

The crystalline structures of the supported catalysts were revealed through the powder XRD technique using SEIFERT 2000 diffractometer operating with CuK_α radiation (λ = 0.1540 nm) generated at 35 kV and 30 mA. Scans were recorded at 1° min^{-1} for 2θ values between 2 to 90 degrees, whereas the peak profile of the (220) reflection of Pd face-centered-cubic (f.c.c) structure (from 62° to 75) was also recorded at the very low scan rate of 0.5° min^{-1} and fitted to a Rietveld algorithm optimizes [1] by using 'Fullprof Suite Program (Version 2.05), so that the position of the peak maximum (θ_{max}) could be obtained precisely degree for alloying calculations. The peak position (θ_{max}) is obtained from curve fitting by using 'Fullprof Suite Program (Version 2.05)' software and used for the calculation of lattice parameter (Equation 1).

$$a = \frac{\sqrt{2}\lambda_{K\alpha}}{\mathrm{Sin}\theta_{max}} \qquad (1)$$

The fitted curve and their corresponding reliability factors (R-factors) have been included in Figure S1 and Table S1 respectively.

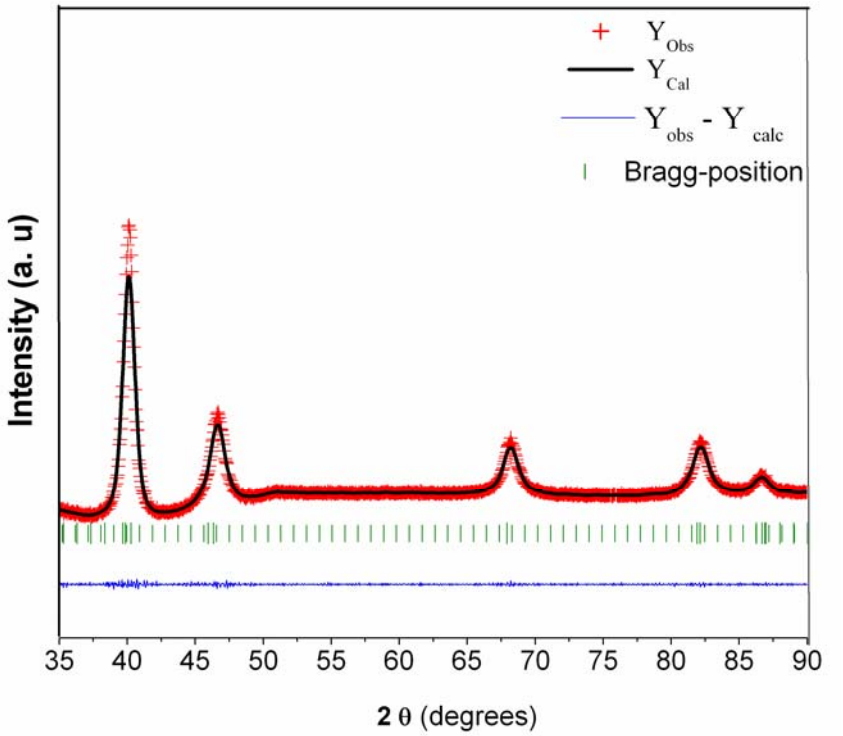

Fig. S 1: X-ray diffraction patterns fitted using the whole pattern profile matching method

Electro-catalysts	Lattice Constant (nm)	(220) diffraction FWHM (deg)	R-factors R_p, R_{wp}, R_p, R_I, R_F
$Pd_{58}Ni_{42}/C$	0.38891± 0.00002	1.35255±0.00003	R_p =1.29 R_{wp} =1.73 $R^{//}_p$=1.81 R_I =1.87 R_F =2.19
$Pd_{37}Ni_{63}/C$	0.38731± 0.00001	1.33101±0.00003	R_p =1.89 R_{wp} =2.33 $R^{//}_p$=2.59 R_I =2.66 R_F =2.93
$Pd_{21}Ni_{79}/C$	0.38613± 0.00001	1.31273±0.00001	R_p = 2.13 R_{wp} = 2.57 $R^{//}_p$= 2.65 R_I = 2.78 R_F = 2.99

Table S 1: Lattice constant and FWHM of (220) phase of synthesized catalyst

Chronoamperometric Study:

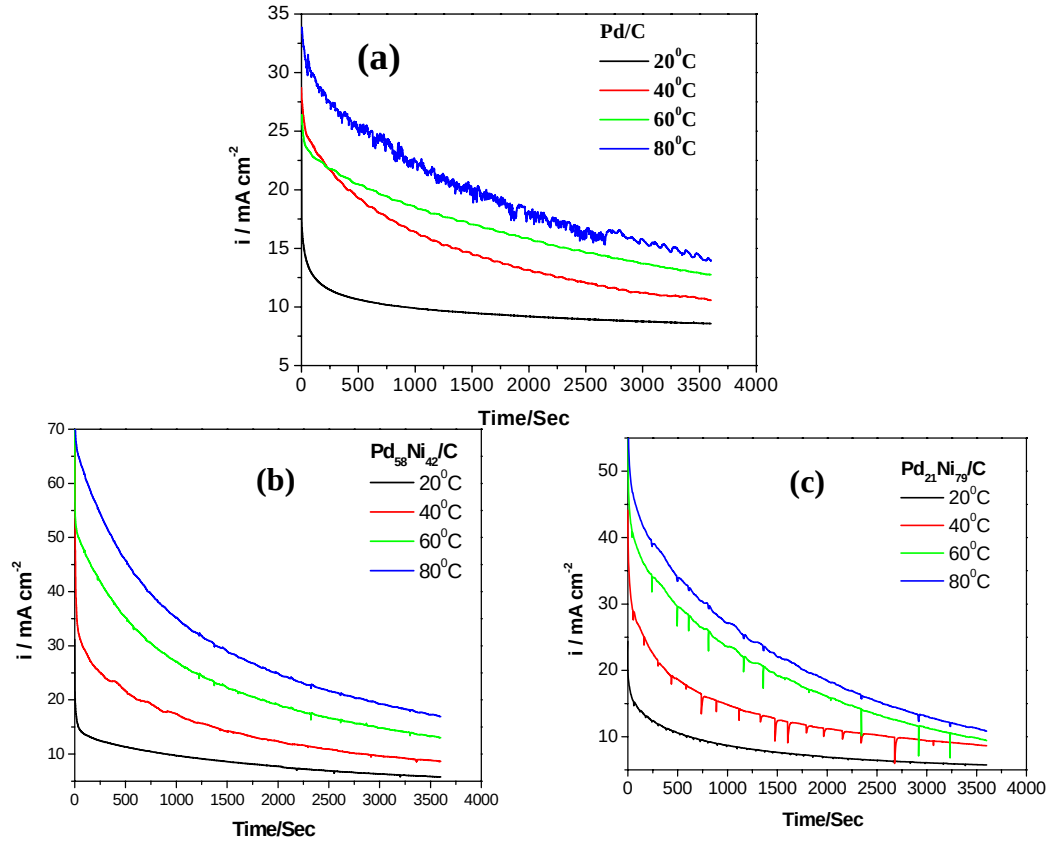

Fig.S2. Chronoamperometric studies of ethanol oxidation on **(a)** Pd/C **(b)** $Pd_{58}Ni_{42}/C$ **(c)** $Pd_{21}Ni_{79}/C$ electrodes at a constant potential of –300mV (vs. Hg.HgO) at different temperatures

Impedance Spectroscopy:

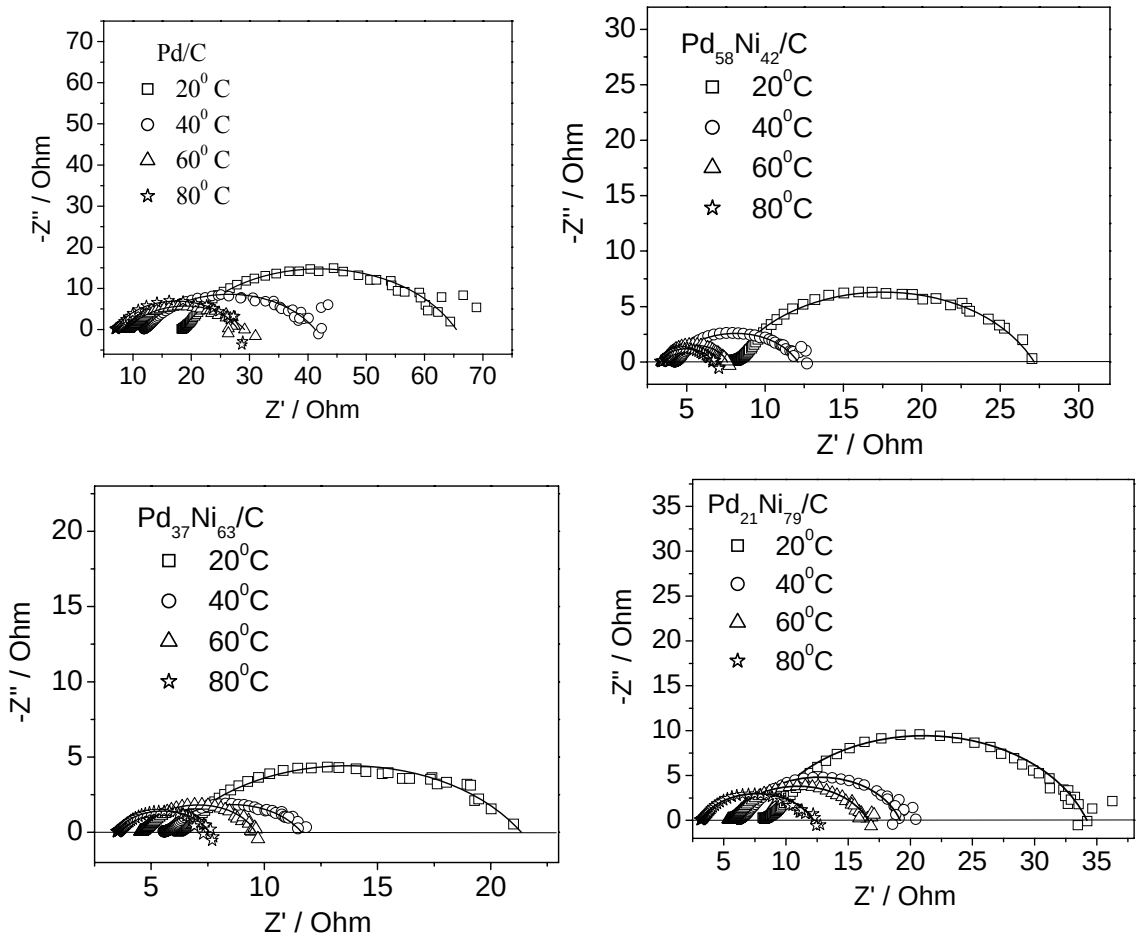

Fig. S3: Nyquist plots of ethanol oxidation in 0.5 M NaOH + 1.0 M EtOH at –0.3 V for (a) Pd/C (b) $Pd_{58}Ni_{42}$ (c) $Pd_{37}Ni_{63}$ (d) $Pd_{21}Ni_{79}$ at different temperatures.

References:

[1]. B. Tobey, *Int. Centre for Diffraction Data*, *Powder Diffr.,* 2006, 21, 67-70