Supporting information

Effect of the reaction parameters on the size and composition of Pt-Sn nanoparticles prepared by the polyalcohol reduction method

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The lattice parameter, calculated from each reflection by using the

$d_{hkl}=\frac{n\lambda}{2\sin\Theta}$ and $a_{exp}= d_{hkl}\sqrt{(h^2+k^2+l^2)}$ equations for the alloys with the fcc structure.

For the hexagonal system the following equation valid between the lattice spacing and the lattice constants:

$$d_{hkl}=\frac{1}{\sqrt{\frac{4}{3a^2}(h^2+k^2+l^2)+\left(\frac{l^2}{c^2}\right)}}$$

By using the *100, 200, 300* reflections (k=0, l=0) the equation above can be simplified and the lattice parameter a can be determined by the following formula:

$$a=d_{h00}*h*\sqrt{\frac{4}{3}} \qquad \text{for } h=1,2,3.$$

The corresponding d_{h00} values were calculated by using the Bragg equation based on the measured 2Θ values of the *h00* reflections of the sample.

The calculated lattice parameter (a_{exp}) corresponding to each crystal planes was plotted versus

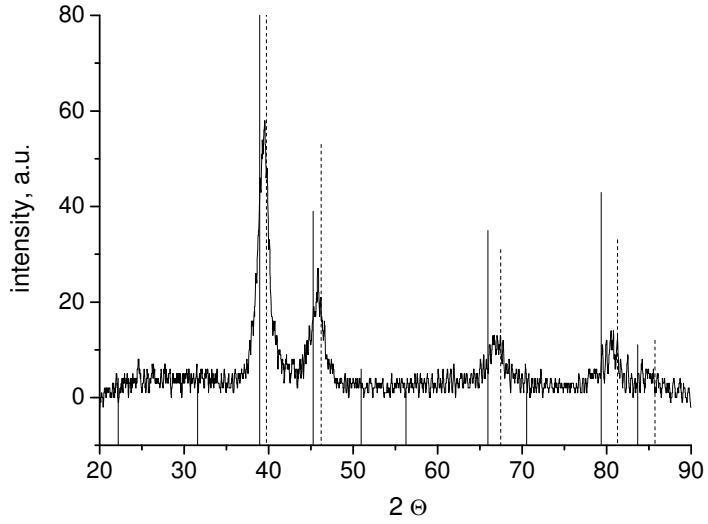
$$x = \frac{1}{2}\left(\frac{\cos^2\Theta}{\sin\Theta} + \frac{\cos^2\Theta}{\Theta}\right).$$

The extrapolation of the linear fit to the zero value of the abscissa gives the lattice parameter.

The following data were used for the Nelson-Riley plot presented in Figure 3.

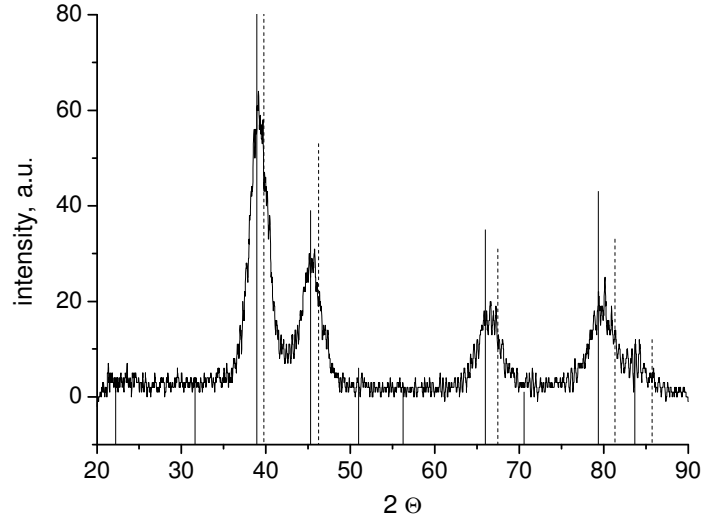
			Pt_3Sn (35-1360)					
h	k	l	2 theta	theta	theta rad	d hkl (A)	a exp (A)	x
1	1	1	38.946	19.473	0.340	2.3104	4.0017	2.641
2	0	0	45.270	22.635	0.395	2.0013	4.0025	2.185
2	2	0	65.970	32.985	0.576	1.4147	4.0014	1.257
3	1	1	79.354	39.677	0.692	1.2063	4.0010	0.892

			Pt (04-0802)					
h	k	l	2 theta	theta	theta rad	d hkl (A)	a exp (A)	x
1	1	1	39.765	19.8825	0.347	2.2647	3.9225	2.574
2	0	0	46.244	23.122	0.404	1.9613	3.9227	2.125
2	2	0	67.456	33.728	0.589	1.3871	3.9234	1.210
3	1	1	81.289	40.6445	0.709	1.1824	3.9217	0.848



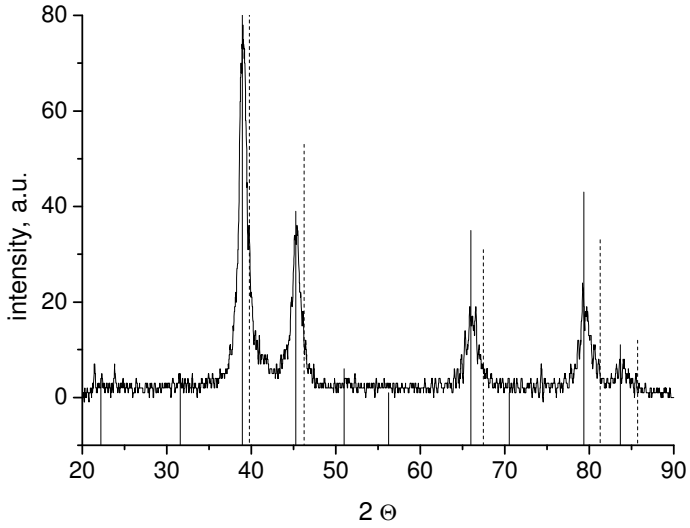
Reference patterns: solid line Pt_3Sn, dotted line Pt

			Sample No. 10					
h	k	l	2 theta	theta	theta rad	d hkl (A)	a exp (A)	x
1	1	1	39.411	19.7055	0.344	2.2842	3.9564	2.603
2	0	0	45.752	22.876	0.399	1.9813	3.9626	2.155
2	2	0	66.845	33.4225	0.583	1.3983	3.9550	1.229
3	1	1	80.452	40.226	0.702	1.1926	3.9555	0.866



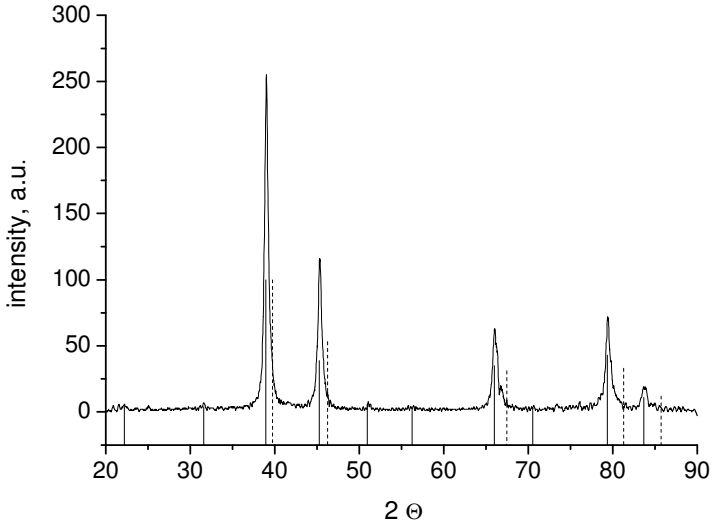
Reference patterns: solid line Pt_3Sn, dotted line Pt

			Sample No. 4					
h	k	l	2 theta	theta	theta rad	d hkl (A)	a exp (A)	x
1	1	1	39.199	19.5995	0.342	2.2961	3.9769	2.620
2	0	0	45.367	22.6835	0.396	1.9972	3.9944	2.179
2	2	0	66.467	33.2335	0.580	1.4053	3.9749	1.241
3	1	1	79.825	39.9125	0.697	1.2004	3.9813	0.881



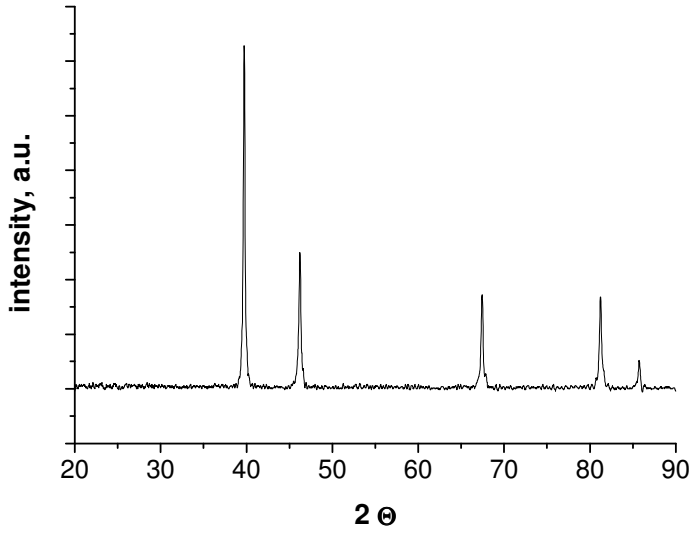
Reference patterns: solid line Pt_3Sn, dotted line Pt

			Sample No. 7					
h	k	l	2 theta	theta	theta rad	d hkl (A)	a exp (A)	x
1	1	1	39.059	19.5295	0.341	2.3040	3.9906	2.632
2	0	0	45.318	22.659	0.395	1.9992	3.9985	2.182
2	2	0	66.185	33.0925	0.578	1.4106	3.9899	1.250
3	1	1	79.539	39.7695	0.694	1.2040	3.9932	0.887

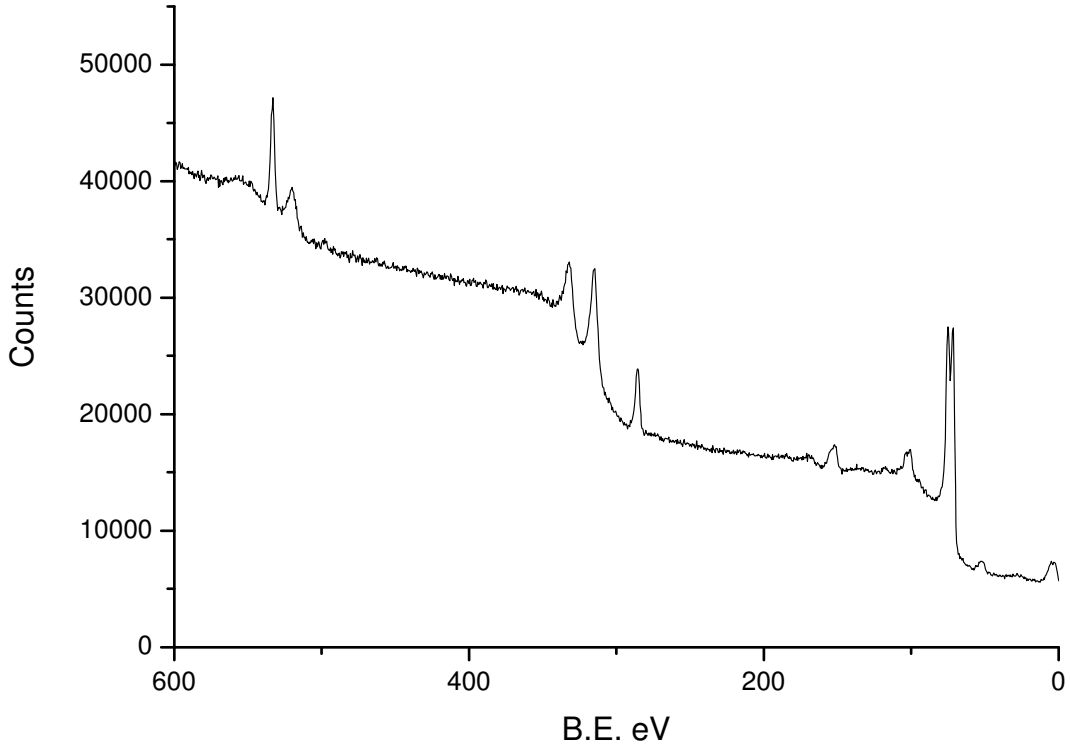


Reference patterns: solid line Pt_3Sn, dotted line Pt

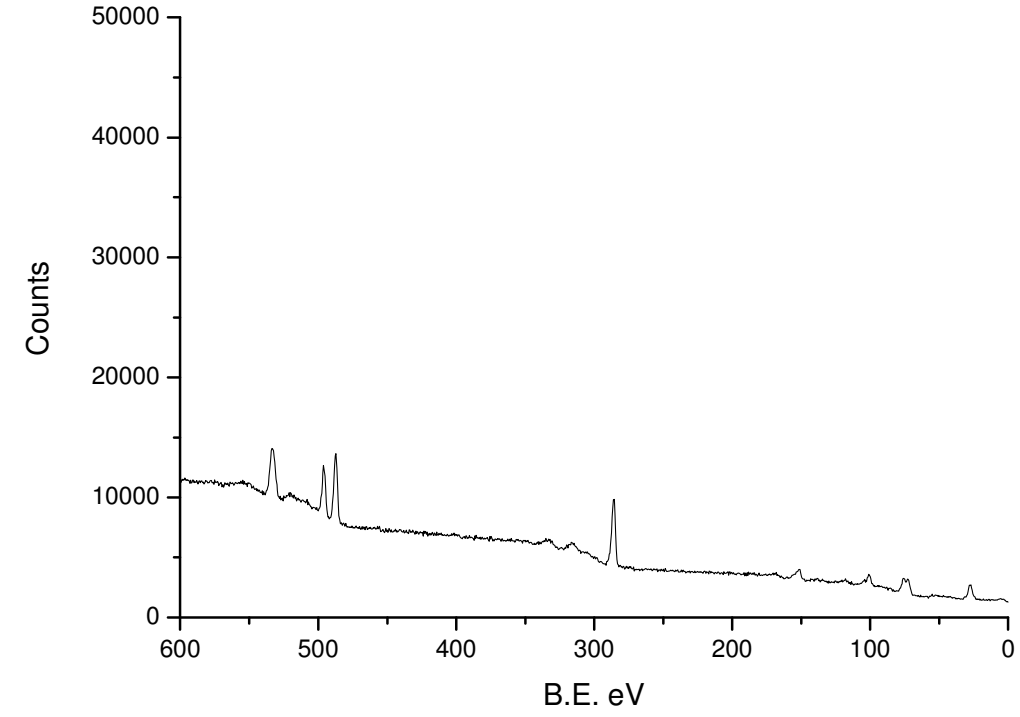
			Sample No. 9					
h	k	l	2 theta	theta	theta rad	d hkl (A)	a exp (A)	x
1	1	1	39.036	19.518	0.341	2.3053	3.9929	2.633
2	0	0	45.354	22.677	0.396	1.9977	3.9955	2.180
2	2	0	66.087	33.0435	0.577	1.4125	3.9951	1.254
3	1	1	79.457	39.7285	0.693	1.2050	3.9967	0.889



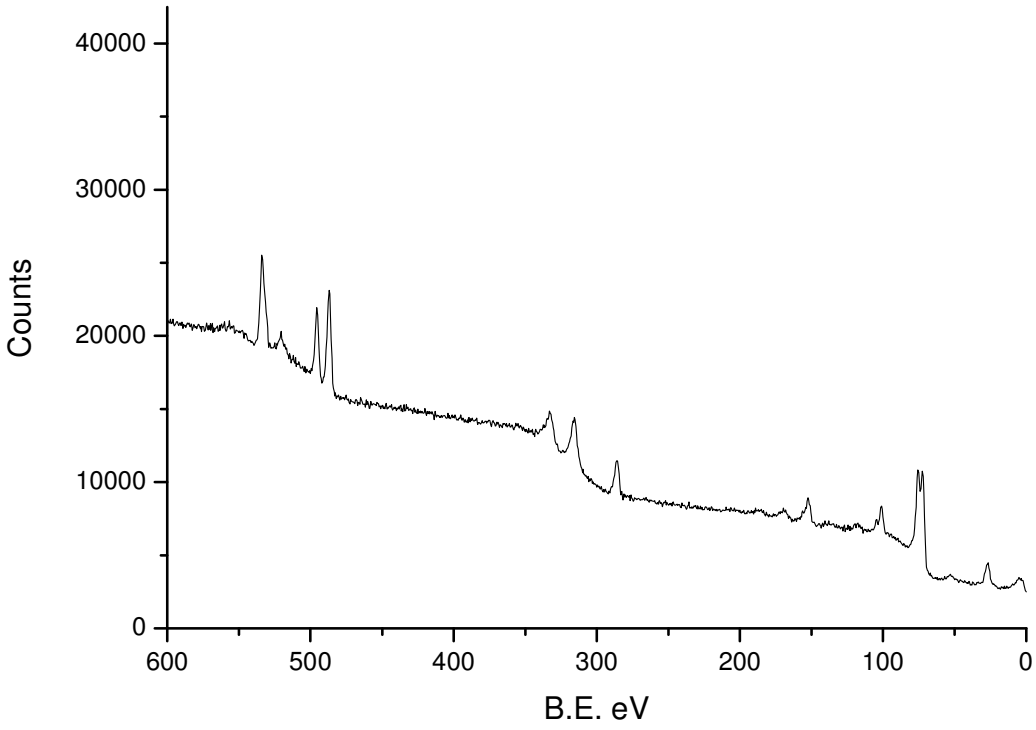
XRD pattern of Pt sample prepared for reference in the absence of capping agents.
Average crystallite size: 33.8 nm
T_R=290 °C. heating rate 5 °C/min. Pt: 0.0973g. (0.24 mmol). 0.574 g 1.2-hexadecanediol.
solvent: octyl ether. 20 ml.



XP survey spectrum of Pt sample prepared in the absence of capping agents.



XP survey spectrum of sample 15. (PtSn).



XP survey spectrum of sample 8. ($Pt_{0.86}Sn_{0.14}$).