Electronic Supplementary Material (ESI) for CrystEngComm

Supporting information

for

One-step solvothermal synthesis of nickel selenide series: composition and morphology control

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Rietveld refinements of $NiSe_2$

The Rietveld method was used to refine the XRD patterns of $NiSe_2$. The profile function used for describing the peak shape was a Pseudo-Voigt type and the background was modeled as a polynomial. The crystallographic data and the details of Rietveld structure refinement are collected in Table S1.

Table S1. The results of Rietveld refinement of $NiSe_2$ samples

Data evaluation	Source	a (Å)	b (Å)	c (Å)	V (nm^3)	z	D (g/cm^3)	R_p (%)	R_{wp} (%)	wt% orthor-homb-ic	wt% cubic
Rietveld	Cu target	4.9049(2)	5.9727(5)	3.6752(1)	0.1075(4)	2	6.7430	7.29	9.98	100.0	0.0
Rietveld	Cu target	4.9145(1)	5.9635(7)	3.6815(9)	0.1078(9)	2	6.7904	8.89	10.67	77.9	22.1
		5.8453(6)	5.8453(6)	5.8453(6)	0.1997(2)	4					
Rietveld	Cu target	4.9149(1)	5.9582(1)	3.7336(5)	0.1033(6)	2	6.8012	6.78	10.12	29.1	70.9
		5.9544(3)	5.9544(3)	5.9544(3)	0.2110(5)	4					
Rietveld	Cu target	5.9576(2)	5.9576(2)	5.9576(2)	0.2114(6)	4	6.8043	6.09	9.12	0.0	100.0

Figure S1 showed the corresponding electron diffraction patterns, which matched the structures of cubic $NiSe_2$ (JCPDS no. 41-1495), orthorhombic $NiSe_2$ (JCPDS no. 18-0886) and hexagonal NiSe (JCPDS no. 18-0888). It indicated that the samples were well crystallized.

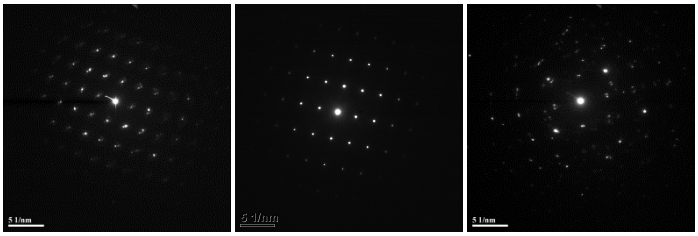

Figure S1. The corresponding electron diffraction patterns of cubic $NiSe_2$, orthorhombic $NiSe_2$ and hexagonal NiSe.