Supplementary Material (ESI) for CrystEngComm

(111) Twinned $BaTiO_3$ Microcrystallites

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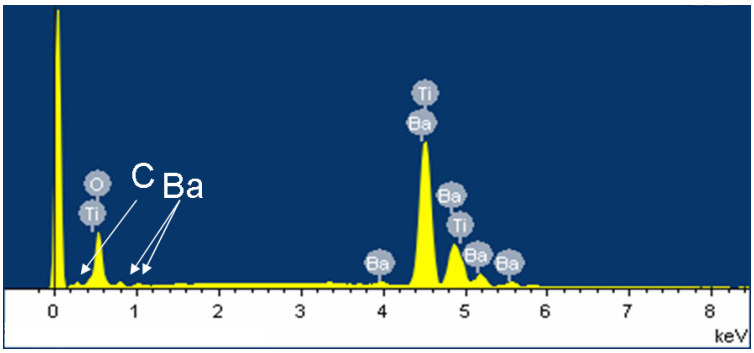

Figure S1. EDS result of the product synthesized at 180°C for 20 days.

Figure S1 shows the EDS result. It can be seen that the sample contains only barium, titanium and oxygen. It is confirmed that the as synthesized product is $BaTiO_3$. The small peak of carbon is from the conductive tape used for sample mounting.

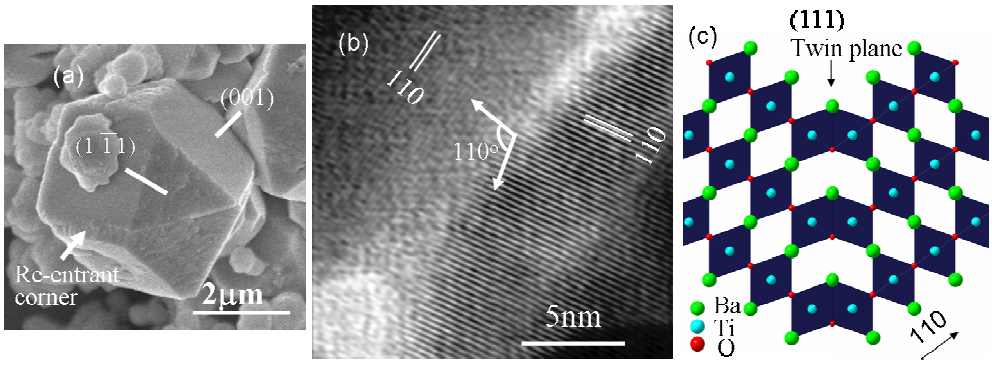

Figure S2. SEM image (a) and HRTEM image (b) of $BaTiO_3$ particle synthesized at 180°C for 1day. (c) Schematic drawing of the (111) twin interface in the $(1\bar{1}0)$ projection.

A typical (111) twinned $BaTiO_3$ particle can be found in Figure S2a. The exposed faces can be readily identified as the (001) and $(1\bar{1}1)$ faces. Re-entrant corners can also be identified, as marked in the figure. The HRTEM lattice image of a (111) twin is shown in Figure S2b. The (110) directions of the two individuals can be identified by FFT (d(110) = 0.28nm), which form an angle of 110°, in agreement with the crystallographic aspects of (111) twins (Figure S2c).