Mild, Facile Synthesis of Perovskite Oxynitride Nanoparticles Towards High-entropy Thermoelectric Materials

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Currently commercially available thermoelectric (TE) materials – which can convert directly from a temperature difference to an electric current – have high conversion efficiency (represented by the *ZT* value), but make use of toxic or rare elements. In contrast, oxides, including perovskites, are known to be non-toxic and stable to high temperatures.[1] However, their *ZT* values are low due to poor electrical conductivity, large band gap[2] and high thermal conductivity. Increasing *ZT* generally involves the introduction of dopant elements such as La, Bi or Pb, which harms the sustainability of such materials.[3] In this research, we focus on the synthesis of highly sustainable perovskite nanoparticles for future application as TE materials.

$SrTiO_3$ nanoparticles (NPs) (Fig. 1) were synthesized using a mild, facile gel-sol method, followed by characterization by XRD, TEM, EDS, XPS, and UV-vis. Synthesis also included the introduction of different alloying elements, such as Ca and Mn, to the Sr and Ti sites. The introduction of multiple alloying elements is known to increase the configurational entropy, leading to benefits such as significantly reduced thermal conductivity. Following the synthesis of alloyed $SrTiO_3$ NPs a nitridation step was performed by mixing with urea at mild temperatures to substitute a portion of the O atoms with N and thus reduce the optical band gap.[4] The produced oxynitride NPs had a measured indirect optical band gap of 2.2 eV, significantly reduced from the 3.1 eV of the $SrTiO_3$ NPs.

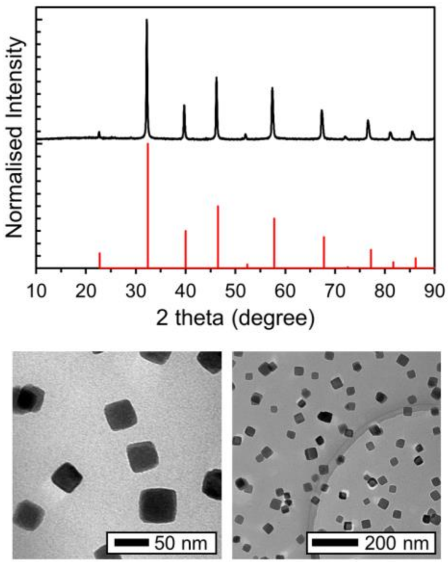

Figure 1: XRD pattern and TEM images of as-synthesised $SrTiO_3$ NPs. Red is the reference pattern for cubic $SrTiO_3$ (PDF: 00-005-0634)

References
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