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Fabrication of Sub-Stoichiometric Ti2O3 for Room Temperature Thermoelectric Energy Regeneration: Tuning of Structural and Electronic Properties via Defects Engineering

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Titanium oxides has drawn extensive attention as functional electronic materials in the past few years, due to their unique layered structure and physical properties. Sub-stoichiometric titania are particularly interesting non-toxic materials for thermoelectric applications because of their high electrical conductivity with possible low phonon thermal conductivities originated from phonon scatterings at ordered defect planes. Hereby, layered sub-stoichiometric Ti2O3 material has been successfully fabricated by densifications of the ball-milled precursors with spark plasma sinterings. The experiments were performed on densified Ti2O3 samples with 0.5, 3 and 10 h ball-milling times to compare the changes in PDOS. The application of high-energy ball milling could significantly decrease the grain size in the SPS-densified bulk sample, and thus affect the phonon behaviours. The XRD results showed with the increasing of ball milling hours, the percentage of Ti3O5 increased while Ti2O3 is still the main phase. Measurements of phonon density-of-states (PDOS) were performed with the PELICAN time-of-flight neutron spectrometer in the energy-gain mode at ANSTO, at 200, 300, 500 and 650 K, respectively. The overall shapes of the GDOS are very similar across the three samples, with three peaks located at around 20, 40, and 60 meV and matched well with the calculated PDOS of Ti2O3, indicating the dominate phase for three samples are still Ti2O3. With the temperature increasing, the peak intensity at around ~20 meV increased, however, the red-shifts and intensity decreases were observed at the 40 and 60 meV phonon DOS peaks (as indication of anharmonic effects). This suggested that the acoustic phonons response differently to temperature increase compared to optical phonons. The intensities at between 50 to 60 meV increases for the 10H spectrum, compared to the other two. This is probably because of the excitation of the phonon states in Ti3O5, as the increased Ti3O5 percentage in 10H sample. Our results suggested the measurement matched well with the theoretical study, which indicates the structural changes could have played significant roles in determining the phononic structure of sub-stoichiometric Ti2O3 based material.

Topic

Physics

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