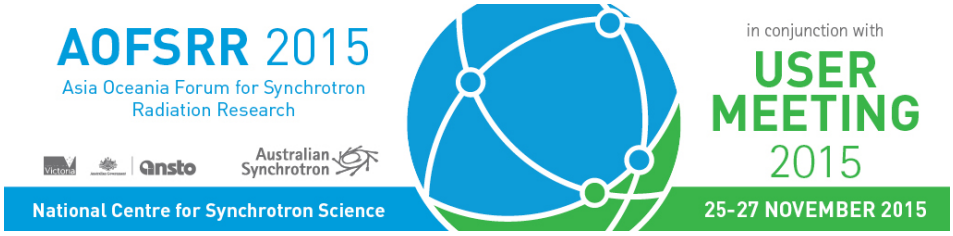

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Activation energies for phase transformations in electrospun titania nanofibers: comparing the influence of argon and air atmospheres

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The paper reports the way in which titania absolute phase levels (amorphous, anatase and rutile forms) in electrospun amorphous titania nanofibers change with temperature over the range 25–900 ℃ according to the controlling environment for calcination as the material is heated non-isothermally. The environments chosen for study were air and argon. A novel method was developed to extract the absolute levels of amorphous titania and crystalline anatase and rutile from the synchrotron radiation diffraction (SRD) data. Determination of absolute phase levels facilitated estimation of the activation energies for the amorphous-to-anatase transformation, 45(9) kJ/mol in argon and 69(17) in air; and for the anatase-to-rutile transformation energies, 97(7) kJ/mol for argon and 129(5) for air. An activation energy estimate for amorphous-to-crystalline titania in argon, 142(21) kJ/mol using differential scanning calorimetry (DSC) is consistent with the SRD results. The differences between the activation energies for heating in air and argon are attributed to the presence of substantial oxygen vacancies when the material is heated in argon. Estimates of anatase and rutile oxygen site occupancies from the SRD data show that (i) anatase has discernible oxygen vacancies in argon between 700–900 ℃ corresponding to the stoichiometry TiO2-x with x < 0.4; (ii) the anatase stoichiometry in air at these temperatures is TiO2; and (iii) rutile does not have significant oxygen vacancies in either argon or air between 800–900 ℃.

Keywords

Electrospun titania nanofibers; Anatase; Rutile; Activation energies; Oxygen vacancies.

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