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Visible and IR photoluminescence of c-FeSi@a–Si core–shell nano-fibres produced by vapour transport

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Abstract

The procedures for the synthesis of amorphous ε-FeSi/Si core–shell nanofibres by vapour transport in a CVD configuration are reported. Crystallite studies by the Williamson-Hall method show the sizes to be typically about 8.0nm which agrees with TEM value of 7.9nm fibre diameter with a compressive strain of about 0.04. Features in the photoluminescence of these FeSi core–shells in both visible and IR are at 10nm, 1062nm, 1414nm and 1772nm and absorption feature at 1000cm^{-1} from FTIR are explained from density functional theory (DFT) ab initio calculations. PL confirms the intra-band transition whereas FTIR agrees perfectly with the band-to-band transition whose band gap energy is 0.13eVforFeSi. FTIR also unveils inter-band transition which DFT calculation could not predict. Raman spectroscopy data confirm FeSi and nano-Si presence.