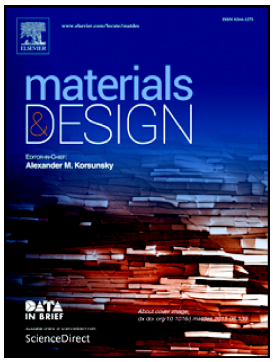

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Influence of pulsed-electric-current sintering conditions on the non-stoichiometry and thermoelectric properties of $Ti_{1+x}S_2$

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Abstract
Nearly stoichiometric $Ti_{1.005}S_2$ was prepared by a solid-state synthesis of the constituent elements and consolidated under a variety of processing conditions applied using pulsed-electric-current sintering. The non-stoichiometry in the $Ti_{1+x}S_2$ induced during the sintering was quantitatively determined with a Rietveld structural refinement and a thermogravimetric analysis combined with inductively coupled plasma atomic emission spectroscopy. Significant cation off-stoichiometry and sulphur losses were already observed at a sintering temperature of 700 °C, resulting in heavily self-intercalated $Ti_{1.076}S_2$, which significantly altered the thermoelectric properties in comparison with the nearly stoichiometric compound. By applying a high sintering pressure of 500 MPa the $Ti_{1.005}S_2$ could be consolidated at 500 °C with no detectable sulphur loses and with a high bulk density of 97.6 %. The sulphur volatilization in the TiS_2 was also effectively suppressed up to 800 °C by using a gas-tight sintering mould, which resulted in the composition $Ti_{1.017}S_2$, prepared at 800 °C and 200 MPa, with an optimal thermoelectric figure of merit ZT equal to 0.32 at 375 °C.

Keywords: Titanium disulphide, Thermoelectric materials, Pulsed electric current sintering, Structure-property relationship, Transport properties

Highlights:

- Sintering TiS_2 can result in off-stoichiometry and the intercalation of Ti atoms.
- Such structural changes greatly affect the thermoelectric properties of TiS_2.
- S/Ti ratio decreases with sintering temperature upon the volatilization of sulphur.
- Highest S/Ti ratio is obtained by high-pressure sintering at lower temperatures.
- Sulphur volatilisation is restrained when using a gas tight-sintering mould.

Introduction

The research on novel materials for energy conversion is essential for the development of sustainable, renewable and environmentally friendly energy technologies. Among the viable approaches, solid-state thermoelectric (TE) devices with no moving parts, high reliability and scalability have led to a worldwide interest in their use for waste-heat recovery and refrigeration [1]. Thermoelectric technology is based on materials that directly convert a heat flux into electrical energy (and vice