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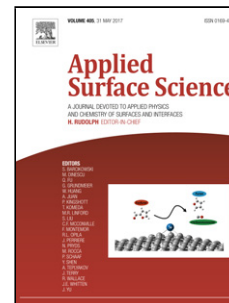
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# Lithium Intercalation Studies in Cubic Titanium Carbide Thin Films

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## Abstract

In this study, titanium carbide (TiC) was deposited using reactive magnetron sputtering onto copper substrates. Sputtering was done at room temperature while in the presence of methane. Formation of crystalline cubic TiC as confirmed by x-ray diffraction (XRD). A discharge capacity of  $169 \mu A h g^{-1}$  was observed for the Cubic Phase TiC thin film/Lithium half-cells. Cyclic Voltammetric studies showed that the reduction reaction of the half-cell occurred at 0.78 V, while the oxidation reaction occurred at 1.1 V. Charge/discharge cycles showed a decrease in discharge capacity when the half-cell was cycled between 0.01 and 3.0 V. X-ray Photoelectron Spectroscopy (XPS) analysis of the Li intercalated TiC films showed that cubic phase TiC, hydroxyl groups, titanium sub oxides and lithium fluoride compounds were formed. The crystallite size of the cubic TiC was of the order of 15 - 20 nm.

*Keywords:* Titanium Carbide, XPS, XRD, SEM, Thin Film Battery, Lithium

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## 1. Introduction

Lithium ion thin film batteries are of predominant interest to the consumer electronics industry and the emerging electric transportation sector. Favorable properties such a high energy density, low self discharge rate, the absence of memory effects, a wide operational window and a relatively longer lifespan make it viable for manufactures to adopt lithium ion thin film batteries. In recent years, batteries have also been viewed as a bridge between the electricity grid and renewable energy generation. A highly developed lithium ion thin film battery system integrated along with solar and wind farms could aid electricity grids to cope with fluctuating energy supply and demand. The present generation of lithium-ion batteries use graphite carbon as a negative electrode and layered transition metal oxides such as (LiCoO<sub>2</sub>) or phosphates (LiFePO<sub>4</sub>) as positive electrodes. This generates a net energy density of a 100 - 150 Wh/kg (cell capacity 70 mAh/g) [1]. The major limitation of a thin film battery would be the need for a stable electrode that has a high energy density as well as a relatively high lifetime. Research is currently advancing towards employing metallic anode materials that possess higher capacity. Metallic anode materials allow the intake and release of Lithium via alloying and de-alloying, forming inter-metallic compounds or solid solutions with lithium during electrochemical cycling [2]. Several researched electrode materials have been considered undesirable for the reasons pertaining to volume expansion, high processing temperatures, poor adhesion to the substrate and poor electronic conductivity [3, 4]. Due to the low intercalation/deintercalation potentials and favorable reversible capacities of metal carbides with respect to lithium metal, there has been an interest in developing metal carbide electrode materials for lithium based batteries [5].

Advanced alloy anodes have been developed with a long life cycle of over 300 cycles and a reversible capacity of 500 - 700 mAh/g. The capacity fade rates of these alloy materials are as low as 0.07% per cycle. Simultaneously, the first-cycle irreversible capacity loss of alloy anodes can be reduced to 50 - 100 mAh/g, corresponding to a high initial coulombic efficiency of  $\approx 90\%$ . The cause of first-cycle capacity loss has been attributed to a loss of active material, solid electrolyte interface formation, Li trapping in the host alloy, reaction with oxide impurities and the aggregation of active particles [6]. The Scientific basis of mechanical and electrical properties of transition metal carbides are very well reported in the literature for both bulk and thin film form [7, 8, 9, 10]. Transition metal carbides are a new class of materials for energy storage and catalysis application [11, 12]. Transition metal carbides are of interest due to their electronic properties.

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