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## Reactive Chemical Vapour Deposition of titanium carbide from $H_2$ - $TiCl_4$ gas mixture on pyrocarbon: A comprehensive study

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### Abstract

In Reactive Chemical Vapour Deposition (RCVD), the absence of one element of the deposited carbide in the initial gas phase involves the consumption/conversion of the solid substrate. In this way, the growth of a continuous carbide layer on the substrate requires solid-phase diffusion of the reagent.

In this work, a parametric study of the RCVD of titanium carbide from pyrocarbon (PyC) and an  $H_2$ - $TiCl_4$  mixture has been carried out. Conversion ratio, PyC consumption and carbide layer growth kinetics have been determined at 1000°C. The influence of the  $H_2$ / $TiCl_4$  dilution ratio has been also investigated. The apparent inter-diffusion coefficient of the carbon through the TiC deposited layer and the direct apparent reaction rate were determined from a comparison between simulations based on a Deal-Grove-type model and the experimental results. The study has been completed with FTIR spectrometry analyses of the gases.

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**Keywords:** CVD ; R-CVD ; TiC coating ; pyrocarbon ; solid state diffusion ; FTIR ; simulation

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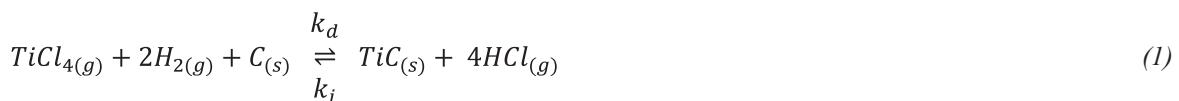
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Nomenclature	
$k_d$	Direct rate constant ( $\text{mol} \cdot \text{m}^{-2} \cdot \text{s}^{-1}$ )
$k_i$	Inverse rate constant ( $\text{mol} \cdot \text{m}^{-2} \cdot \text{s}^{-1}$ )
$r$	Dilution ratio of $\text{TiCl}_4$ in $\text{H}_2$
$x$	Carbon content in the TiC
$D_C$	Solid-state apparent inter-diffusion coefficient of carbon in TiC ( $\text{m}^2 \cdot \text{s}^{-1}$ )
$D_{\text{TiCl}_4}$	Gaseous diffusion coefficient of $\text{TiCl}_4$ ( $\text{m}^2 \cdot \text{s}^{-1}$ )
$p_{\text{TiCl}_4,s}$	$\text{TiCl}_4$ partial pressure on the deposition surface (Pa)
$p_{\text{TiCl}_4,\infty}$	$\text{TiCl}_4$ partial pressure in the RCVD reactor (Pa)
$p_{\text{H}_2,\infty}$	$\text{H}_2$ partial pressure in the RCVD reactor (Pa)
$v_r$	Reaction (1) rate ( $\text{mol} \cdot \text{m}^{-2} \cdot \text{s}^{-1}$ )
$j_C$	Carbon flux from the PyC layer across the deposited TiC layer ( $\text{mol} \cdot \text{m}^{-2} \cdot \text{s}^{-1}$ )
$j_{\text{TiCl}_4}$	$\text{TiCl}_4$ flux from the bulk of the reactor across the limit diffusion layer ( $\text{mol} \cdot \text{m}^{-2} \cdot \text{s}^{-1}$ )
$V_{m,C}$	Carbon molar volume ( $\text{m}^3 \cdot \text{mol}^{-1}$ )
$V_{m,\text{TiC}}$	TiC molar volume ( $\text{m}^3 \cdot \text{mol}^{-1}$ )
$c_0$	Reference concentration of the TiC ( $1/V_{m,\text{TiC}}$ ) ( $\text{mol} \cdot \text{m}^{-3}$ )
$a_i$	Interfacial activity of carbon (interface between TiC and PyC)
$a_s$	Carbon activity in the gas phase near the reaction surface
$R$	Perfect gas constant ( $\text{J} \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$ )
$T$	Temperature (K)
$\theta$	Temperature (°C)
$\delta$	Limit diffusion layer (m)
$P_0$	Reference pressure (Pa)
$R_{v,th}$	Theoretical conversion ratio
$R_{v,ap}$	Apparent conversion ratio
$e_{\text{TiC}}$	TiC thickness (meters for the modeling part and nanometers for the experimental part)
$e_{\text{C, cons}}$	PyC consumed thickness (nm)
$e_{\text{C, ini}}$	Initial PyC layer thickness (nm)
$e_{\text{C, res}}$	Residual PyC layer thickness (nm)

## 1. Introduction

Titanium carbide (TiC) is a frequently studied material for nuclear (Groot et al., 1991) and aerospace engineering applications (Boving and Hintermann, 1990). This material is extremely hard, has good corrosion resistance and refractoriness and is highly electrically conducting. These characteristics made him a good material for being studied.

The Reactive Chemical Vapour Deposition (RCVD) method is used to form carbide coatings and allows thin, homogeneous and adherent layers to be obtained. For instance, carbides (HfC, TiC ...) and boro-carbides (B<sub>4</sub>C ...) from metals of groups 4 and 5 have been deposited for barrier applications in refractory ceramics (Piquero et al., 1995, Baklanova et al., 2006). These authors mentioned that RCVD coating are thin, homogeneous and adherent. The purpose of this work was to study the RCVD of titanium carbide from pyrocarbon according to the overall reaction (1).



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