

유기금속 화학증착에 의한 크롬 카아바이드 코팅에서
탄소 혼입에 관한 열화학적 및 실험적 연구
(Thermochemical and Experimental Study of Carbon Incorporation
in Chromium Carbides Coatings Processed by MOCVD)

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Mono- or poly- phased chromium carbides thin films, more or less contaminated by free carbon, were deposited by Metalorganic Chemical Vapor Deposition (MOCVD) using bis(benzene)chromium, BBC, $\text{Cr}(\text{C}_6\text{H}_6)_2$ as precursor under different experimental conditions. The experimental results, specially the C-incorporation have been compared to a thermochemical study of the deposition process. This theoretical approach consisted of minimizing the Gibbs free energy of the chemical system C-Cr-H-He. This showed the importance of the total pressure and the initial molar fraction of BBC on the composition of the films. Trends predicted by thermochemical calculations are in agreement with the experimental results. Nevertheless, systematic excess of carbon was thermochemically predicted compare to the experiments. This discrepancy has been attributed to a gas phase decomposition of BBC and to a dominant role of the adsorption of the benzene molecules. Subsequently, by adding a small amount of C_6Cl_6 in the reactive mixture, the C-incorporation in the films has been suppressed (~2% at C) confirming that the presence of chlorinated hydrocarbons in the reactants inhibits the dehydrogenation reaction of aromatic ligands.