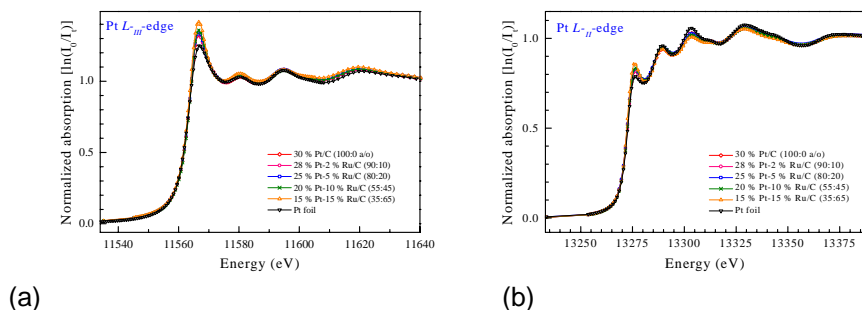


Analysis of Local Structure in Nano-sized Catalysts of Fuel Cells

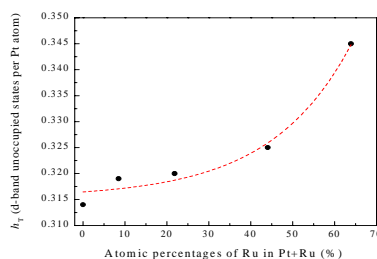
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Abstract:

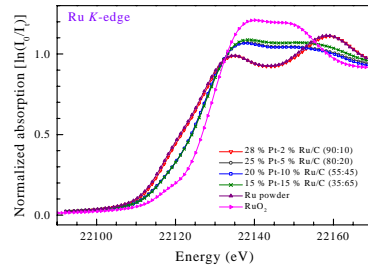
The main goal of this work is to study the effects of the composition of the nano-sized bimetallic particles on the structural and electronic properties of the catalysts. All samples were synthesized by the incipient-wetness impregnation method using an aqueous mixture solution of H_2PtCl_6 and RuCl_3 (or MoCl_5) to yield selected atomic ratio and 30 wt. % of total metal loading. The differences between the energy values corresponding to normalized absorption value of around 0.5 can usually be used to compare the valance of the metal. Therefore, according to the chemical shift of the XANES (X-ray absorption near edge structure) spectra, Pt in the PtRu/C (as shown in Fig. 1) and PtMo/C catalysts (not shown here) are metallic while both Ru and Mo in PtRu/C (or PtMo/C) are oxidized with the edge positions shifted positive to their corresponding metal powder (as shown in Fig. 3 and 4). The estimated values are about 2+ and 4+ for Ru and Mo, respectively. These results indicate that both Ru and Mo have affinity for the absorption of O_2 or H_2O in air at room temperature. The results of XANES spectra analysis at the Pt L_{III} and L_{II} edge are illustrated in Fig. 2 and 5. Although Pt are determined as metallic state and alloyed with Ru and Mo (based the XRD analysis), the amounts of d-band vacancy are always much than that of Pt foil. It means that some Pt 5d electrons overlap with the lower energy level 4d-bands of Ru or Mo when the PtM alloy formed. However, the different extent of changing in the total number of Pt 5d-band vacancy was found. It is believed that the chemical composition of the active sites Pt on the surface of catalysts plays a very important role on the mechanism and efficiency of the catalytic reactions.



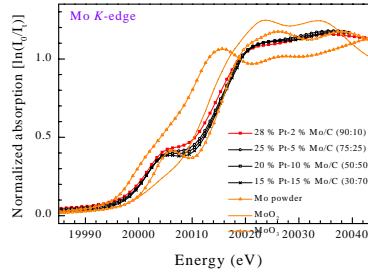
圖一 (a)與(b)分別為不同 Pt/Ru 比例觸媒與鉑箔之 Pt L_{III} -edge 與 L_{II} -edge XANES 圖譜。



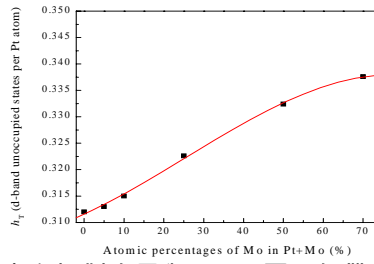
圖二 Ru 於雙金屬系統中之相對含量與 Pt 5d 電子能帶中電子空缺率之關係圖。



圖三 不同 Pt/Ru 比例觸媒與標準物 (Ru 粉末與 RuO₂) 之 Ru K-edge XANES 圖譜。



圖四 不同 Pt/Mo 比例觸媒與標準物 (Mo 粉末、MoO₂ 與 MoO₃) 之 Mo K-edge XANES 圖譜。



圖五 Mo 於雙金屬系統中之相對含量與 Pt 5d 電子能帶中電子空缺率之關係圖。

