

Heritage from Professor An Pang Tsai to the research field of metallic catalysis materials

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We had collaborated exciting themes in materials science together with Professor An Pang Tsai for 17 years (since 2002). Prof. Tsai began the investigation of catalytic materials in term of metallurgy at NIMS [1].

There are three important topics in the collaborative research with Professor Tsai. Firstly, we succeeded that novel catalytic materials were prepared by the leaching method of Al-Cu-Fe quasicrystalline (QC) [2]. The $\text{Al}_{63}\text{Cu}_{25}\text{Fe}_{12}$ QC is a promising precursor for Cu catalysts, whose constituent elements, compositions and quasi-periodic structure are in favor of processing high performance catalysts. Brittleness resulting from quasi-periodic structure enables one to obtain powder form for processing catalysts. Relatively low dissolution rate of Al due to quasi-periodic structure upon leaching with NaOH solution, generated homogeneous nanocomposite consisting of Fe_3O_4 and Cu and hence gave rise to high activity and thermal stability for steam reforming of methanol. Secondary, Prof. Tsai proposed a concept for a pseudo-element material such as “PdZn = Cu” [3]. A clear correlation between electronic structure and CO_2 selectivity for steam reforming of methanol (SRM) was obtained with PdZn, PtZn, NiZn, and PdCd intermetallics on the basis of experiments and calculations. PdZn and PdCd also exhibited valence electronic densities of states and catalytic properties similar to that of Cu. Thirdly, a new concept of active sites for bulk-type metallic materials was proposed by Prof. Tsai, *i.e.*, nano twin boundary [4]. According to the DFT calculation, surface density of the active six-coordinated atoms in nano porous gold (NPG) was comparable with that of supported gold nanoparticle catalysts. In addition, the energy profiles of reaction pathways for CO oxidation indicated that the six-coordinated sites created by twinning significantly contributed to the catalytic activity of NPG. I will overview of these topics in my presentation.

Two years have passed since Professor A.P. Tsai passed away. Taking over Prof. A.P. Tsai's spirits, now we are conducting research on novel metallic catalysis materials under the new system. We hope that those concepts of Prof. Tsai's will lead to a principal for the development of metallic functional materials as well as metallic catalysts in the future.

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- [2] For example T. Tanabe, S. Kameoka, M. Terauchi and A.P. Tsai, “Microstructure of leached Al-Cu-Fe quasicrystal with high catalytic performance for steam reforming of methanol”, *Applied Catalysis, A*, **384** (2010) 241-251.
- [3] A.P. Tsai, S. Kameoka and Y. Ishii, “PdZn=Cu: Can an intermetallic compound replace an element?”, *J. Physical Soc. Jpn.*, **73** (2004) 3270-3273.
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