

In-situ microscopic study of surfaces of intermetallic compounds for catalysis

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Intermetallic complex compounds [1, 2] are of great interest because of their potential and facile catalytic activity for energy and green applications. However the structure and stability of the surfaces is crucial respectively for determining catalytic activity and feasibility for applications. In spite of study of complex metallic alloys and intermetallics over decades, the understanding the surface structure and their stability remains a challenge because of structural complexity. In these class of materials, often, surface atoms are found to have smaller co-ordination number in the surface planes in contrary to the fact that the denser surface-termination are thermodynamically favored in elemental crystal systems. Here we will present results obtained in our recent studies on structures and stability of the surfaces of ZnPd employing scanning tunneling microscopy (STM) and low-energy electron microscopy (LEEM) experiments. The complementary density functional theory (DFT) calculation, DFT-based thermodynamic computation and mathematical modeling were employed to understand mechanism stabilizing surfaces observed in experiments. Among bimetallic compound ZnPd compound was found to be potential for methanol steam reforming [2]. Beside the activity of surfaces, we have found spontaneous surface termination of low-indexed/less compact planes in randomly oriented polycrystalline ZnPd samples. Such low-indexed/less dense surface termination is not seen in single elemental metallic system. The mechanism stabilizing low indexed surfaces of ZnPd might be general for stabilizing the structure of complex intermetallic alloys and will further move us forward to develop understanding of stabilizing mechanism in more general structure such as non-periodic ordered structures.

[1] J. A. Rodriguez, *Surf. Sci. Rep.* **24**, 223-287 (1996).

[2] M. Armbrüster et al., *Catalysis Reviews: Science and Engineering*, **55**, 289 (2013).