In-situ XRPD analysis of thermal stability of catalyst for ammonia synthesis based on cobalt molybdenum nitrides

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Caesium or potassium promoted cobalt molybdenum nitride Co_3Mo_3N obtained via ammonolysis from cobalt molybdate hydrate is more active in ammonia synthesis process than the commercial multi-promoted iron catalyst [1]. The admixture of alkali metals has a beneficial effect on the activity of the catalyst but at the expense of a less developed porous structure and lower thermal stability [2]. Despite the high activity, the application of cobalt molybdenum nitrides in the industry is limited by their low operational parameters, like thermal stability and activity maintenance during the long catalytic process. Development of an efficient strategy to counteract this adverse effect is a critical factor to further applications of cobalt molybdenum nitrides.

Double promotion with potassium and chromium results in the formation of more active and stable material [3]. Chromium is considered a structural promoter, which enhances surface stability and increases the specific surface area of the catalyst. In this study, the thermal stability of the catalyst during the ammonia synthesis process was carefully examined via *in-situ* X-ray powder diffraction (XRPD) studies. Simulation of conditions similar to these applied in the industrial practice was conducted. Furthermore, prolonged heat treatment to simulate the ageing of the catalyst was performed and the stability of the catalyst under a hydrogen atmosphere was examined.

Cobalt molybdenum nitrides occur in three stable crystallographic forms Co_3Mo_3N, Co_2Mo_3N and Co_6Mo_6N. Co_3Mo_3N is isostructural with η-Fe_3W_3C (η-*6* carbide structure); Co_2Mo_3N is isostructural with the filled β-manganese structure; Co_6Mo_6N is isostructural with Fe_6W_6C (η-*12* carbide structure).

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References

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