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Molybdenum carbide nanoparticle: Understanding the surface properties and reaction mechanism for energy production towards a sustainable future

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ABSTRACT

Rational design and synthesis of cheap, noble metal-free, thermal/hydrothermal stable and active catalyst for efficient hydrogenation and hydrogen production reaction is crucial towards renewable and sustainable energy generation. This gives the use of molybdenum carbide nanoparticle considerable attention as an alternative to noble metals. However, the industrial application is not yet feasible due to insufficient stability and activity coupled with the lack of detailed understanding of the reaction mechanism. This work discusses the effect of the operating parameters on the properties and morphology of molybdenum carbide nanoparticle, as well as their impact on the catalytic activity. Critical issues such as structural diversity, surface properties, and multiscale reaction modeling are also discussed for better understanding of the reaction mechanism. This is a promising strategy towards synthesis of cost-effective and efficient catalysts for renewable and sustainable energy production.

1. Introduction

One of the most important research gaps in the field of renewable and sustainable energy is rational design and synthesis of suitable eco-friendly and cost-effective catalysts with preserved energy and chemical functionality for prolonged applications in several industrial processes [1–3]. The unique chemical and physical properties of molybdenum carbide nanoparticle [4] have enhanced its popularity in the fields of materials and chemical science towards production of renewable and sustainable energy [5]. The outstanding properties of MCN include thermal stability, high electrical conductivity, adsorption capacity, high melting point, and hardness [6]. Moreover, the characteristics of MCNs such as resistance to nitrogen and sulfur, high catalytic current density, and durability are similar to those of noble metals, which enable their utilization in hydrogenation and hydrogen evolution reactions (HER) [7,8]. Examples of these reactions include CO_2 hydrogenation to alcohol, CO hydrogenation to alcohol [9], hydrodeoxygenation [10], electrocatalytic hydrogen evolution from water splitting [11] including oxygen evolution reaction [12], hydro-treating [13], watergas shift reaction (WGS) [14], hydrodesulfurization (HDS) [15], CH_4 aromatization [16], and hydrodenitrogenation (HDN) [17]. The MCNs are also suitable for electrocatalytic reactions.

MCN has been used successfully to hydrogenate feedstock such as cellulose, indole, toluene, and cumene, which are popularly processed with group 9 and 10 noble metals (Pt, Pd, Rh) [18–20]. These being commercially available catalysts for reactions such as methane reforming, hydrocarbon isomerization, water-gas shift reactions, and CO hydrogenation. Further, MCN has been employed as an alternative to Ru, and to an extent Pt as electrocatalysts in the anode of polymer membrane fuel cells (PEMFC) [21–23] because of its platinum-like behaviors [24]. The thermal stability of MCN in the absence of oxygen is due to the delay of the sintering and attrition effects as reaction proceeds. However, the catalytic activity of MCN systems mainly depends on the nature and physiochemical properties of the catalyst.

Previously, the high temperature classical metallurgical process was used to prepare metal carbides but the products exhibit low specific surface areas and high particle size [25]. This results in the Metal carbide products exhibiting low catalytic performance in targeted catalytic processes [3]. Currently, the MCN synthesis method by Lee et al. [26], which is a temperature program reduction (TPR) carburization is most popular due to its remarkable improvement on the textural property of the product [27]. TPR carburization is a carbothermal reduction method that carburizes the Mo precursor supported on carbon in hydrogen atmosphere [28]. The Mo precursor is to be thermally treated, at increasing the controlled temperature in a reducing environment [29]. To form the carbide phase, the carbon source is mainly

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Nomenclature

CVD	Chemical vapor deposition
DFT	Density functional theory
DFTB	Density functional tight-binding
EAM	Embedded atom type
ELM	Extreme learning machine
Fcc	Face-centered cubic
Hcp	Hexagonal closest-packed
HDN	Hydrodenitrogenation
HDS	Hydrodesulfurization
HER	Hydrogen evolution reactions
IMLS	Interpolating moving least squares
JCPDS	Joint Committee on Power Diffraction Standards
MCN	Molybdenum carbide nanoparticle
MM	Molecular mechanical
MSI	Modified Sheppard interpolation
NN	Neural-network
PES	Potential energy surface
QM	Quantum mechanical
RKHS	Kernel Hilbert space
RPBE	Revised Perdew–Burke–Ernzerhof
RT	Room temperature
t_{carb}	Carburization time
T_{carb}	Carburization temperature
TMC	Transition metal carbides
TPH	Temperature-programmed hydrogenation
TPR	Temperature program reduction
US	Umbrella sampling
WGS	Watergas shift reaction

light hydrocarbon, while hydrogen is the reducing agent. The essence of the controlled temperature is to optimize the carburation temperature to avoid sintering of the reduced Mo particles, thereby reducing the particle size of the resulting carbide. The carburization conditions (temperature and time) control the physiochemical properties, the chemical nature, and structure of the resulting carbide phase. MCN exists in two main crystalline structures: orthorhombic and hexagonal (Mo_2C) and hexagonal structure. The preparation methods of carbide-supported metal catalysts include wet impregnation [30], atomic layer deposition [31] and vacuum environment [32]. Mostly, the synthesized MCN, passivated prior to its exposure to air to prevent oxidation.

The goal of this review is to provide insight into the surface properties of MCN and its reaction mechanism for renewable and sustainable energy production towards a sustainable future. In Section 2, rational design and synthesis of MCN are discussed, highlighting the effect of operating parameters. The third section deals with a structural diversity of MCN using density functional theory (DFT) to categorize different form of MCN based on structural differences. Section 4 briefly discusses the surface properties of MCNs to determine the stability based on their structural diversity. While Section 5 gives an insight into multiscale reaction model on MCNs for a better understanding of catalytic reaction mechanism of the system, which is crucial to the commercial applications of MCN in the production of renewable and sustainable energy. Finally, we presented the catalytic activity of MCN based catalysts (both unsupported and promoted/supported) in Section 6.

2. Preparation of MCN

MCNs are popularly prepared by carbothermal reduction carburization process. This process consists of three different steps; (i) deposition of the Mo-precursor on the carbon source, (ii) carbothermal reduction of the Mo-precursor to produce MCN, and [33] the subsequent stabilization of the produced MCN by Mo-carbide surface passivation [19]. Generally, synthesis of MoO_2 nanoparticles is not a difficult task; the transformation into MCN is where the major challenge is. The transformation is so complex due to the influence of several variables. Experimentally, different kind of MCN is prepared using various strategies. These strategies include direct carburization of MoO_3 by 10–20% CH_4–H_2 mixtures at 750 °C for 4 h to produce thermodynamically stable hexagonal Mo_2C [34]; reduction of MoO_3 by NH_3 to produce Mo_2N and then carburization of Mo_2N by using CH_4–H_2 mixture to produce orthorhombic Mo_2C [35] reduction and carburization of belt-shaped α-MoO_3 by using 5% *n*-C_4H_{10}–H_2 mixture at 700 °C for 4 h to produce metastable phase face-centered cubic (fcc) α-MoC_{1-x} [36]; solid-state reaction in combination with H_2 reduction at 800z °C to form hexagonal Mo_2C at 20 min reduction time and hexagonal η-MoC at 10 min reduction time using glucose as the carbon source [37]. However, carburization with a 10% C_2H_6–H_2 mixture produces in mixed crystal phases [36]. All the phases can be differentiated and identified with ease. MCN can also be synthesized via reactive hard-templating, a technique where a precursor such as $MoCl_5$ is used with mpg-C_3N_4 as a template in ratio 1:1 in ethanol solution (Eq. (1)) [38].

$$(MoCl_5 + 2C_2H_5OH \rightarrow MoCl_3(OC_2H_5)_2 + 2HCl) \quad (1)$$

Furthermore, Hare et al. [39] and Saito et al., [40] used arc discharge method to prepared β -Mo_2C and α-Mo_2C encapsulated with polyaromatic carbon. The most efficient and common strategy for MCN production is high temperatures reduction and carburization of MoO_3 by a mixture of hydrocarbon and hydrogen. The major advantages of this strategy are the formation of a pure crystal phase and avoidance of contamination by coke. Typically, the crystalline phase can be controlled by reconciling the gas composition of the reducing and carburizing agent [41]. However, the effect of the operating parameters has not been significantly explored. The synthesized MCN normally possess random size distribution, which ranges from few nanometers to several hundred nanometers with irregular shapes [42].

2.1. Effect of operating parameters on the nature of MCN

The effect of carburization conditions such as carbon source, pretreatment temperature T_{preT}, heating rate, Mo loading, carburization time (t_{carb}), carburization temperature (T_{carb}), Mo-precursor and crystalline phases is vital on the MNC crystalline Mo-phases. The effect could be analyzed by comparing the measured H_2-consumption from TPR results and the crystallinity of the carburized samples via XRD analysis.

2.1.1. Carbon source

The morphology of MCN is highly sensitive to the choice of hydrocarbon used. Mo et al. [43] reported that a high concentration of carbon source such as long chain hydrocarbon favors the formation of MoC (with face-centered cubic (fcc)) and nanosized Mo_2C (with hexagonal closest-packed (hcp)) due to the severity of carbon deposition at high carburization temperature. The deposited carbon may block the mesopores to form new micropores [43]. Further, increasing the chain length of the carbon source lessens the particle size and the required carburization temperature for MCN synthesis [41]. The use of low concentration of small chain hydrocarbon leads to agglomeration of carbide particles at a low heating rate. Prominent among the carbon sources are 20% CH_4–H_2 to form hexagonal close-packed MCN, 5% n-C_4H_{10}–H_2 to form fcc MCN, 10% C_2H_6–H_2 to form mixed crystal phases by the reducing and carburizing the precursor. The MCN synthesized with C_2H_6–H_2 as the carburizing agent exhibits the roughest surface and highest adsorption capacity for H_2, while synthesized with n-C_4H_{10}–H_2 exhibits a very condensed surface [41]. Recently, Tang et al. [37]

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