Study on reduction-carburization of MoO₃ to nano Mo₂C

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Transition Metal Carbides (TMCs) have gained considerable attention in industries because of their refractory nature, attractive physical and chemical properties including high hardness, thermal stability and especially their catalytic activities. Among TMCs, molybdenum carbide (Mo₂C) is currently in high demand for catalytic applications because of high chemical stability, good electrical conductivity and surface activity as its electronic structure is similar to noble metals [1, 2]. The replacement of noble metals by cheaper non-precious alternatives would bring valuable savings. Several methods have been employed to synthesize Mo₂C in nano-scale to enhance the catalytic activity. In the present work, nanocrystalline Mo₂C has been synthesized via a simple reduction carburization route using molybdenum trioxide (MoO₃), metallic magnesium powder as reducing agent and acetone (C₃H₆O) as carbon source in an autoclave. Acetone on decomposition not only provides carbon but also hydrogen to facilitate the complete carburization of MoO₃ to Mo₂C [3]. The reduction kinetics has been studied thoroughly. Figure 1 illustrates the formation of Mo₂C via reduction-carburization of MoO₃ in an autoclave.

Figure 1: Schematic illustration of formation of Mo₂C through reduction-carburization of MoO₃

The optimization of reaction parameters has been done to obtain a single phase Mo₂C as different phases are obtained in reduction process. Thermodynamic parameters have been studied for these phases and the condition for optimized one has been analyzed. Table 1

shows the details of various reaction parameters at different synthesis temperatures. Figure 2 shows the XRD analysis of different synthesized samples with variation in reaction temperature. It proved that the complete synthesis process involved reduction-carburization of MoO₃ to Mo₂C. This is because of intermediate lower oxide phase, which helps in reduction of MoO₃ and formation of Mo₂C.

Table 1: Details of reaction parameters

Sample Id →	S-1	S-2	S-3
MoO ₃ (g)	1.4394	1.4394	1.4394
Mg (g)	3	3	3
Acetone (mL)	10	10	10
Temperature (°C)	600	700	800
Holding Time (h)	10	10	10
Rate (°C/min)	5	5	5

Figure 2: XRD pattern of reduction-carburization of MoO₃ to Mo₂C

References

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3. Singla G., Pandey O. P., Ceram. Int. 40, 5157-5164, 2014