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Synthesis mechanism of MoS₂ layered crystals by chemical vapor deposition using MoO₃ and sulfur powdersJi-Hoon Ahn¹, Se-Hun Kwon², Cheol Min Hyun¹, Jeong-Hun Choi¹, Seung Won Lee¹ and Chang-Min Kim²¹Korea Maritime and Ocean University, Republic of Korea²Pusan National University, Republic of Korea

Monolayer MoS₂ layered crystals have attracted significant attention owing to their potential applicability in emerging devices and Chemical Vapor Deposition (CVD) is the best method so far to obtain monolayer MoS₂ single crystals. Although many studies have been published on MoS₂ monolayer crystals grown by CVD, there is a lack of understanding of its synthesis pathway. Therefore, in this study, we investigated the mechanism of the synthesis pathway when monolayer MoS₂ crystals are synthesized by a conventional CVD method using MoO₃ and sulfur powders. By analyzing the synthesized crystals and byproducts, we discovered that MoS₂ crystals are synthesized on a substrate in 2D form by an intermediate phase of solid MoO₂ produced by the reduction of MoO₃ by sulfur, rather than being synthesized directly from vaporized MoO₃ and sulfur. Based on our observations, we propose two possible reaction mechanisms for MoS₂ synthesis by CVD using MoO₃ and sulfur powders. First, MoS₂ crystals could be mainly synthesized via reaction of MoO₂ and sulfur vapors. MoO₃ powder contained in the crucible would be reduced to MoO₂ rather than sulfurized to MoS₂ by sulfur vapor. Then, vaporized MoO₂ could react with sulfur vapor to form MoS₂ crystals on the substrate. Moreover, we found that MoS₂ layered crystals can also be formed from pre-formed MoO₂ crystals on the substrate. The two mechanisms could be occurring concurrently and the role of an intermediate phase of MoO₂ is very important in both processes.

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