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The synthesis and investigation on the reversible conversion of layered ZrS_2 and ZrS_3

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Figure S1. A schematic illustration of the two-step thermochemical H₂S splitting cycle [1].



Figure S2. Schematic illustration of the experimental setup for the synthesis of metal sulfides from sulfur and metal; (a) tube setup without blocking effect, (b) tube setup with self-blocking effect, and (c) a photo of tubular reactor.



Figure S3. Phase diagram of Zr-S binary system in sulfur atmosphere, Zr : Solid_Alpha, Zr(s2): Solid_Beta, S(liq): liquid phase and S(s2): Beta_monoclinic



Figure S4. Diagram for Zr-S system showing the phase conversion of ZrS_3 and ZrS_2 under the experimental condition of N₂ atmosphere (pN₂ = 1 bar at room temperature)



Figure S5: XRD diffraction patterns of vanadium sulfides prepared under atmospheric pressure; 550 °C (a), 650 °C (b), and 750 °C (c)



Figure S6 a. SEM image shows the determination of the width and thickness of nanobelts (a ZrS_3 sample was synthesized at 550 °C with blocking effect)



Figure S6 b. SEM image of ZrS₃ nanobelts synthesized at 550 °C and atmospheric pressure



Figure S6 c. SEM image allows to view nanobelts in a large scale of a ZrS_3 sample that was synthesized at 550 °C with blocking effect



Figure S6 d. SEM image allows to view nanobelts in a large scale of a ZrS_3 sample that was synthesized at 650 °C



Figure S7. The equilibrium compositions of the decomposition reaction of H_2S by ZrS_2



Figure S8. The temperature dependence for the H_2/H_2S partial pressures in the decomposition reaction of H_2S by ZrS_2

References

[1] O. Osasuyi, K. Al-Ali, M. Abu Zahra, G. Palmisano, D. Viet Quang, Material screening for two-step thermochemical splitting of H_2S using metal sulfide, E3S Web Conf., 83 (2019) 01003.