Van der Waals layered $MoSi_2N_4$ materials family

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2D materials, such as atomically thin graphene, hexagonal boron nitride and transition metal dichalcogenides, are normally limited by the known 3D bulk materials. The design and synthesis of entirely new 2D materials, particularly van der Waals (vdW) layered materials, would significantly expand the properties and functionalities of 2D materials.

In 2020, we proposed a general concept to synthesize new 2D vdW layered materials by passivating the dangling bonds of 2D nonlayered crystals with appropriate elements [1]. Building on this concept, we developed a chemical vapor deposition (CVD) method to grow nonlayered 2D transition metal carbides/nitrides with diverse structures [2]. Interestingly, during the CVD growth of 2D molybdenum nitride, the introduction of elemental silicon was found to effectively passivate the surface dangling bonds, leading to the formation of a new vdW layered material, $MoSi_2N_4$ [1]. This monolayer material can be structurally described as a MoN_2 sandwiched between two Si-N bilayers. It exhibits semiconducting behavior with a bandgap of ~1.94 eV, a high theoretical carrier mobility of up to 1200 cm^2/Vs, outstanding mechanical strength (~66 GPa), good thermal conductivity (~173 W/mK), and excellent ambient stability [1,3]. When multilayer MoN was sandwiched between the two Si-N bilayers, a superconducting $MoSi_2N_4(MoN)_{4n}$ homologous compound was formed [4]. Density functional theory calculations further predicted a large family of $MoSi_2N_4$-structured 2D layered materials with the general formula MA_2Z_4 [1,5]. Moreover, wafer-scale growth of $MoSi_2N_4$ and WSi_2N_4 films and the characterization of point defects in these materials have been demonstrated [6,7].

To date, over a hundred MA_2Z_4 materials and their derivatives have been predicted, encompassing metals, semiconductors, superconductors, topological insulators, ferroelectrics, and ferromagnets, due to the diversity of elements and structures in MA_2Z_4 [8]. Such materials exhibit a variety of novel electronic, optical, thermal, mechanical, ferroelectric, electric contact, magnetic and spin-valley properties, as well as promising applications in electronic and optoelectronic devices, electrocatalysis, photocatalysis, and batteries [8].

References

[1] Y. L. Hong, W. C. Ren, et al., Chemical vapor deposition of layered two-dimensional $MoSi_2N_4$ materials, Science 369 (2020) 670-674.
[2] C. Xu, W. C. Ren, et al., Large-area high-quality 2D ultrathin Mo_2C superconducting crystals, Nature Materials 14 (2015) 1135-1141.
[3] C. J. He, W. C. Ren, et al., Unusually high thermal conductivity in suspended monolayer $MoSi_2N_4$, Nature Communcations 15 (2024) 4832.
[4] Z. B. Liu, W. C. Ren, et al., Two-dimensional superconducting $MoSi_2N_4(MoN)_{4n}$ homologous compounds, National Science Review 10 (2023) nwac273.
[5] L. Wang, W. C. Ren, X. Q. Chen, et al., Intercalated architecture of MA_2Z_4 family layered van der Waals materials with emerging topological, magnetic and superconducting properties, Nature Communcations 12 (2021) 2361.
[6] D. Y. Yang, C. Xu, W. C. Ren et al., Wafer-scale and doping-tunable p-type semiconducting monolayer WSi_2N_4 film, National Science Review 13 (2026) nwag191.

[7] J. M. Tong, Z. B. Liu, W. C. Ren et al., Point defects in monolayer WSi_2N_4 and $MoSi_2N_4$, Nature Communcations (2026) https://doi.org/10.1038/s41467-026-70946-7.
[8] T. Y. Zhou, C. Xu, W. C. Ren, The van der Waals $MoSi_2N_4$ materials family, Nature Reviews Materials 10 (2025) 907.

Figures

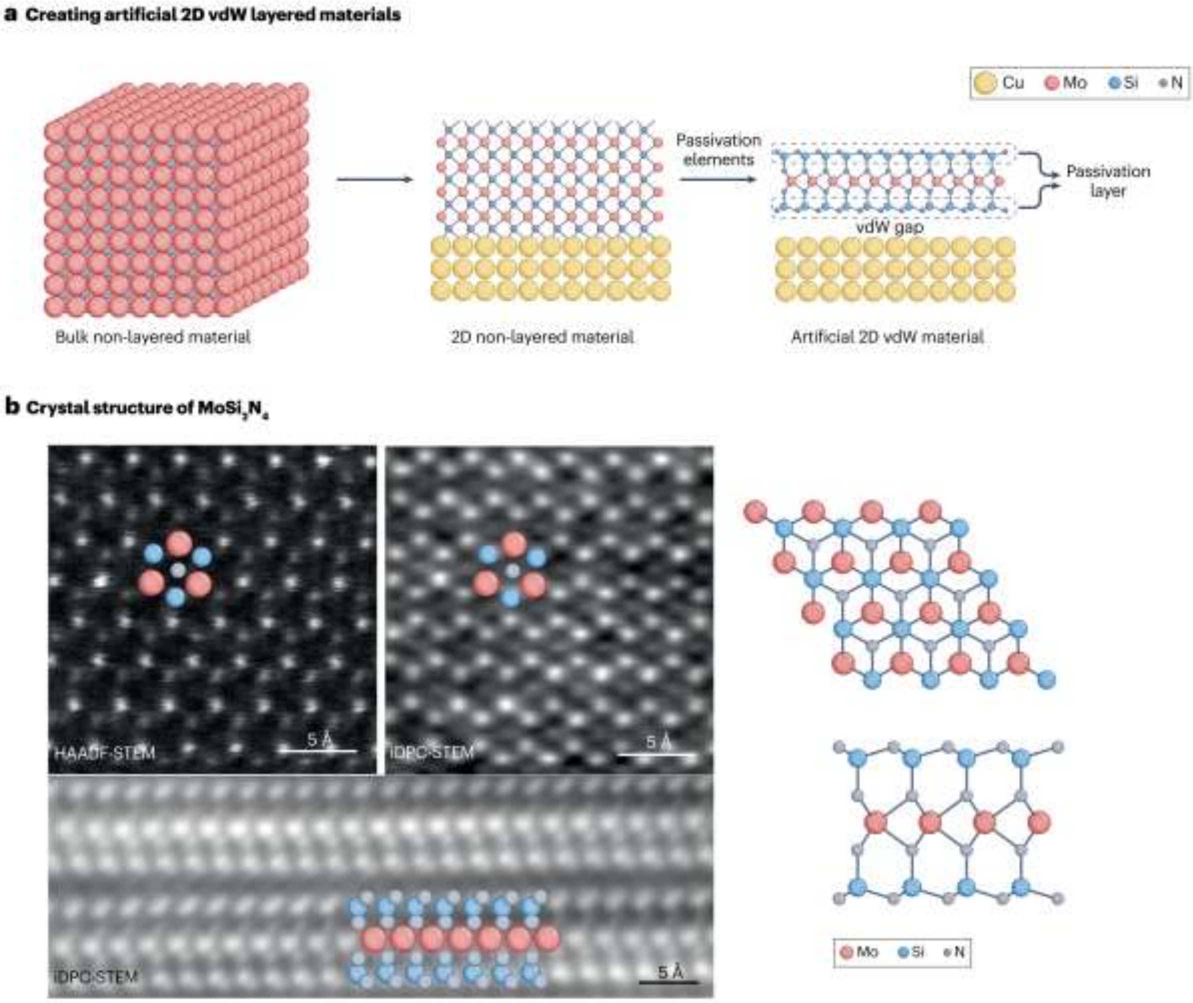

Figure 1: Synthesis and crystal structure of $MoSi_2N_4$