First-Principles Study on Ordered Layers of Metal Melts at Magnetic Solid-Liquid Interfaces

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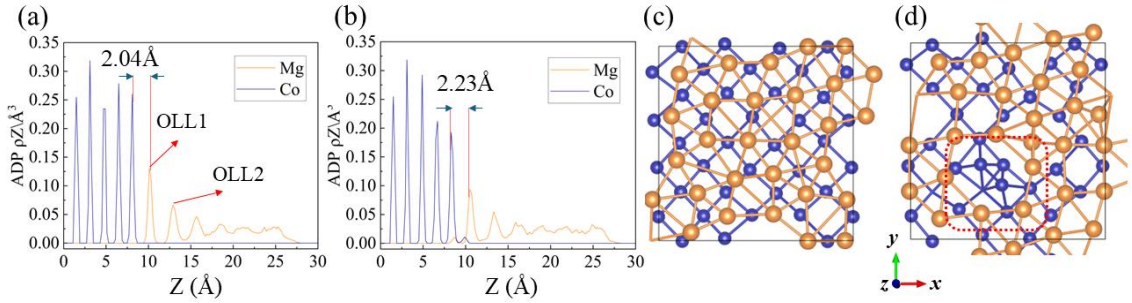
We investigated the magnetic effects at the interface between a ferromagnetic cobalt (Co) substrate and liquid magnesium (Mg), as well as their influence on heterogeneous nucleation, using first-principles molecular dynamics simulations. The study found that Mg atoms at the interface exhibit an induced magnetic moment of approximately 0.02 μB/atom. Magnetism increases the solid-liquid interface distance by about 10%, reduces the atomic order of the ordered liquid layer (OLL1) at the interface, and decreases the coverage (θ) of Mg atoms on the substrate in the OLL1 layer (non-magnetic θ=0.81 vs. magnetic θ=0.75). Additionally, the unique interfacial structure and increased roughness under magnetic influence suggest that magnetism may induce roughening of the solid-liquid interface, thereby affecting the heterogeneous nucleation process. Charge analysis reveals that magnetism suppresses interfacial charge transfer (reduced by 0.15 e/Co atom), leading to weakened Co-Mg interactions (binding energy increases by 0.35 J/m²). This work elucidates the regulatory mechanism of magnetic substrates on the ordered layers at liquid metal interfaces through interface coupling effect, providing a theoretical basis for external field-controlled heterogeneous nucleation.



[1] W. Fu, T. Hu, G. Zhang, S. Qian, W. Xuan, Y. Yang, D. Singh and Z. Ren, Strong Effect of Magnetism at the Cobalt-Magnesium Solid-Liquid Interface, Scripta Materialia (2025) 268, 116892. https://doi.org/10.1016/j.scriptamat.2025.116892