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Liquid/substrate interface for the heterogeneous nucleation in grain refinement of Al alloys

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ABSTRACT

Grain refinement by inoculation is determined by heterogeneous nucleation and crystal growth. The physical process of heterogeneous nucleation on substrates, which depends on the nucleation potency of substrates, is still not fully understood. The present criterion for judging the capability of heterogeneous substrates only concerns the lattice misfit with nucleated crystal. To exactly understand the grain refining mechanism of α-Al by the Al–Ti–B master alloy, the α-Al/solid-TiB_2 and liquid-Al/solid-TiB_2 interfaces were studied using the *ab initio* molecular dynamics. Different ordered structures were formed on the TiB_2 (0001) surface with different terminations, which determines the nucleation potency of TiB_2. Five-layer quasi-solid region with a stacking sequence like fcc-Al (111) forms on the Ti-terminated TiB_2 surface, which is the basis of successful heterogeneous nucleation of α-Al. The reason for using the Al-5Ti-1B master alloy as the commercial refiner in Al industries lies in two aspects: the excessive Ti atoms in the master alloy could guarantee the sufficient Ti chemical potential to form Ti-terminated surface of TiB_2, and the locally stacking reconstruction induced by Ti atom relieves the accumulated elastic strain energy in ordered Al layers, facilitating fully heterogeneous nucleation on substrate. The simulation results were evidenced by the HRTEM and synchrotron XRD.

KEYWORDS: liquid–solid interface, heterogeneous nucleation, grain refinement, *ab initio* molecular dynamics, solidification