Monte Carlo simulations of solute segregation at the liquid-substrate interface

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Grain refinement facilitates the casting process, reduces cast defects and improves the mechanical performance of the final components. One of the most widely used examples of grain refinement is the addition of Al-Ti-B refiners in aluminium casting.

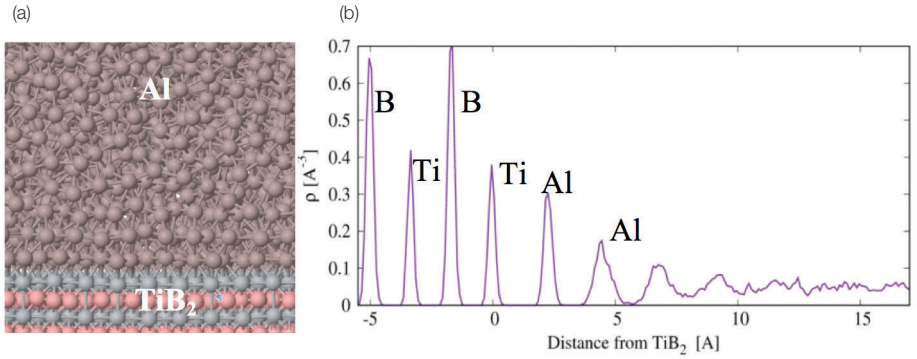

FIGURE 1. (a) A snapshot of the MC simulation of TiB_2-Al at 900 K. (b) The density profile of TiB_2-Al perpendicular to the interface.

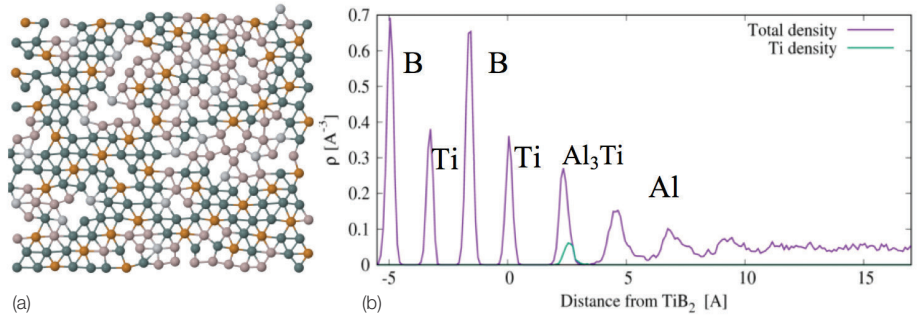

FIGURE 2. (a) The Al_3Ti layer at 1400 K as viewed along the z axis. Atoms are coloured as follows: Blue: ordered Al, Orange: ordered Ti, Pink: disordered Al, Grey: disordered Ti. (b) The density profile of Al_3Ti at 1400 K

Experimental studies of this system have revealed that a single Al_3Ti layer is formed at the interface between the solid TiB_2 and liquid Al [1], and that this layer increases the potency of TiB_2 for heterogeneous nucleation of Al [2]. Motivated by the success of the Al-Ti-B refiner we would like to investigate other liquid/substrate systems in which the segregation of solute and/or impurities will occur. This requires the development of a method to simulate the segregation process. However, this is complicated by the fact that the segregation may happen over long time scales and involve solute concentrations which are very dilute. Consequently, long simulations of large systems containing possibly many thousands of atoms are needed. Such simulations are beyond the capabilities of ab-initio and classical molecular dynamics. Therefore, we have focussed on using monte carlo (MC) simulations.

The aim of this work so far has been to perform MC simulations to understand the segregation of Ti to the TiB_2/Al interface, resulting in the formation of Al_3Ti. In doing so we aim to develop a method that will allow further systems to be studied. As no potential currently exists for the Ti-B-Al system, the initial objective was to produce a Lennard Jones (LJ) potential that will accurately represent the system. This was achieved by fitting the LJ parameters to produce the correct lattice constants and formation energies of various materials such as TiB_2, AlB_2 and TiAl. This was then tested for TiB_2-Al by running a MC simulation of the system at 900 K and comparing the structure to existing ab-initio results [3]. The density profile of the system is shown in Figure 1, which was found to match that produced in [3]. We then determined the stability of an Al_3Ti layer at the interface using this potential. MC simulations were performed at various temperatures and the stability of the Ti atoms in the layer were monitored. We found that the Al_3Ti layer may be stable up to 2000 K. This can be attributed to the fact that the first 3 layers are semi-solid at these temperatures, and there is very little movement of atoms between these layers (Figure 2). However, over longer time scales it may be possible that the Al_3Ti may dissolve.

The next steps are to extend this current method to allow for simulation of larger systems, where low concentrations of the solute can be used in order to reproduce segregation conditions. We also plan to perform MC simulations using the semi-grand canonical ensemble, which allows for compositional changes in the system throughout the simulation. We will then investigate a variety of new systems and determine the ideal conditions for solute segregation.

REFERENCES:

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