Reactive wetting versus non-reactive wetting

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Non-reactive and reactive wetting are the two broad categories of wetting. Many experimental efforts have been made to examine wetting mechanisms, but there are still many questions remain unanswered. Theoretically, non-reactive wetting is fairly well described. However, due to the complexity of the reactive wetting process especially for a highly reactive wetting system like liquid Aluminum (Al) /solid Nickel (Ni) at high temperatures a better understanding of the effect of reactivity on the wetting is needed.

Atomistic simulation can be of great help to better understand mechanisms controlling the wetting process. The main goal is to study non-reactive and reactive wetting of Al(l) on Ni(s) and characterize the effect of reactivity on the wetting.

Molecular Dynamics simulations are performed with Embedded Atom Method force field developed by Zhou et al. (2004). To simulate the wetting, a droplet of Al(l) is positioned on top of a substrate of Ni(s) at 1023.15 K (Figure 1). To simulate a non-reactive wetting system, Ni atoms displacements are restricted to just thermal vibrations.

When in close contact, Ni and Al atoms diffuse into each other. Several consequences are observed: 1) Temperature increases at the interphase due to the exothermic reactions. 2) Different intermetallics form. 3) The composition of substrate and droplet are changing during the wetting. As a result, e.g. droplet properties such as surface tension is changing during the spreading. The effect of reactivity on spreading rate is also explored by modeling the base radius dynamics as $R=at^b$ where t is time. Reactive wetting shows a higher value of b than non-reactive wetting, i.e. reactivity enhances the spreading rate [1].

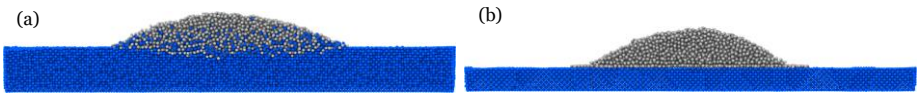

Figure 1. *Side view (Cross-section) illustration of reactive (a) and non-reactive (b) wetting of liquid Al (Gray atoms) on solid Ni (Blue atoms) at 50 ps*

References

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