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Omeje Ilemona, Itina Tatiana

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## Numerical study of early oxidation effects on laser-treated surface

Omeje Ilemona Sunday<sup>1</sup> and Itina Tatiana<sup>1</sup>

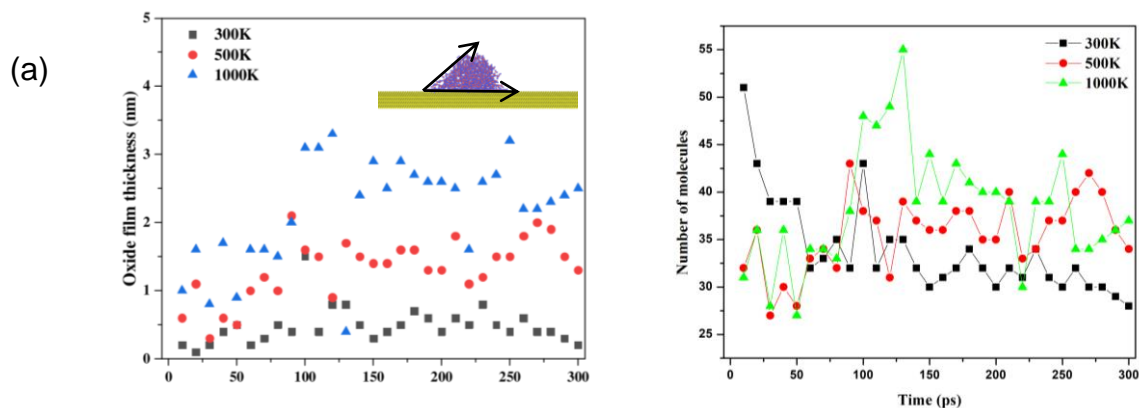
<sup>1</sup>Laboratoire Hubert Curien, UMR 5516, Université Jean Monnet

**Doctorant: Ilemona Sunday OMEJE**

Surface texturing by direct laser ablation creates micro- and nano-scale roughness on materials, resulting in increased surface area and improved surface energy [1]. In particular, micro- and nano-textured surfaces find numerous applications in virus and bacterial repulsion, including the osseo-intergration process in biomedical implants [2]. Laser treatment is one of the most efficient tools for surface texturing, but it can introduce surface oxidation or chemical modifications that cause changes in wettability over time. Despite the significance of these changes, the underlying reasons are not yet fully understood [2–4].

In order to gain further insights into these effects, we performed reactive molecular dynamics (RMD) simulations to understand the effect of early oxidation on laser-treated titanium. The RMD simulations were performed at a temperature of 100K and raised rapidly to 300K, 500 K, and 1000 K, respectively. The obtained results show that oxide thickness increases with time (Fig. 1a). Hence, the  $\text{TiO}_x$  layer grows more quickly in the early stages (0–130 ps) than it does in the later stages (130–300 ps). This condition is brought on by an increase in the  $\text{TiO}_x$  layer and a decrease in  $\text{O}_2$  diffusion (Fig. 2b).

The obtained results are then used in a series of wetting simulations, where in addition to droplet behavior on Ti, the one on Ti with  $\text{TiO}_x$  layer/inclusions are performed. The obtained results show that the presence of oxide makes the droplet behavior less hydrophobic in agreement with experimental observations. Interestingly, because oxide layer thickness rises with time, the contact angle drops down with time [4] and this effect is more pronounced if the surface was heated to a higher temperature [5-6]. Based on this, our calculation sheds light on how the surface wettability of laser-treated materials alternate. The calculated dynamics of the early titanium oxidation correlates with the early time-evolution of laser-treated surface wettability.



**Figure 1** (a) Growth of the oxide film as a function of time; (b) Evolution of the number of molecules of  $\text{O}_2$ , during the oxidation of Ti at 300K, 500K and 1000K. (The insert in Fig. 1a shows our MD simulation results of the surface wettability.)

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