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► **To cite this version:**

Omeje Ilemona, Itina Tatiana E. Itina Tatiana. Numerical study of early oxidation effect on wettability of laser-treated surfaces. 9th Nanotech and Nanomaterials Research Conference, Nano Rome-2023, Jun 2023, Rome, Italy. ujm-04183664

**HAL Id: ujm-04183664**

**<https://ujm.hal.science/ujm-04183664v1>**

Submitted on 19 Oct 2023

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# Numerical Study of Early Oxidation Effect on Wettability of Laser-treated Surface



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## 1.0 Introduction

Surface texturing by direct laser ablation creates micro- and nano-scale roughness on materials, resulting in an increased surface area and surface energy modifications [1]. In particular, micro- and nanotextured surfaces find numerous applications in virus and bacterial repulsion, including the osseointegration process in biomedical implants [2]. However, surface oxidation and other chemical modifications cause changes in wettability over time. Despite the significance of these changes, the underlying reasons are not yet fully understood [2-4]. To gain further insights into these effects, we performed reactive molecular dynamics (RMD) simulations to understand the effect of early oxidation on wettability of laser-treated titanium (Ti) (Fig. 1).

### 1.1 Study Outlook

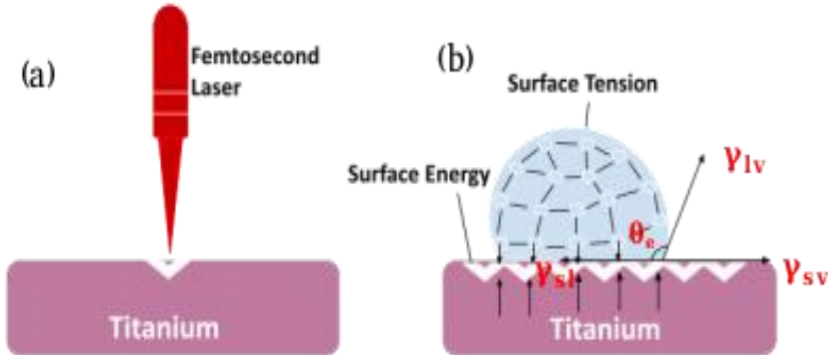


Fig 1. wettability of laser-treated Ti

### 2.0 Computational Details

#### REAXFF Potential

$$BO'_{ij} = BO_{ij}^{\sigma} + BO_{ij}^{\pi} + BO_{ij}^{\pi\pi}$$

$$= \exp \left[ p_{bo,1} \left( \frac{r_{ij}^{\sigma}}{r_o} \right)^{p_{bo,2}} \right] + \exp \left[ p_{bo,3} \left( \frac{r_{ij}^{\pi}}{r_o} \right)^{p_{bo,4}} \right]$$

$$+ \exp \left[ p_{bo,5} \left( \frac{r_{ij}^{\pi\pi}}{r_o} \right)^{p_{bo,6}} \right],$$

Table 1: Model Validation

|                             | LAMMPS  | Experiment           |
|-----------------------------|---------|----------------------|
| a (hcp) (Å)                 | 2.909   | 2.951 <sup>a</sup>   |
| c/a (hcp) (Å)               | 1.588   | 1.588 <sup>a</sup>   |
| E <sub>coh</sub> (kcal/mol) | -115.04 | -115.00 <sup>b</sup> |

## 5.0 Results and Discussion

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. 4a). Hence, the TiO<sub>x</sub> 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 TiO<sub>x</sub> layer and a decrease in O<sub>2</sub> diffusion (Fig. 2). We subsequently performed the wetting studies on the Ti and TiO<sub>x</sub> (Fig. 3(a)(b)). The obtained results show that the presence of oxide makes the droplet behavior less hydrophobic (Fig. 4a) in agreement with experimental observations [5].

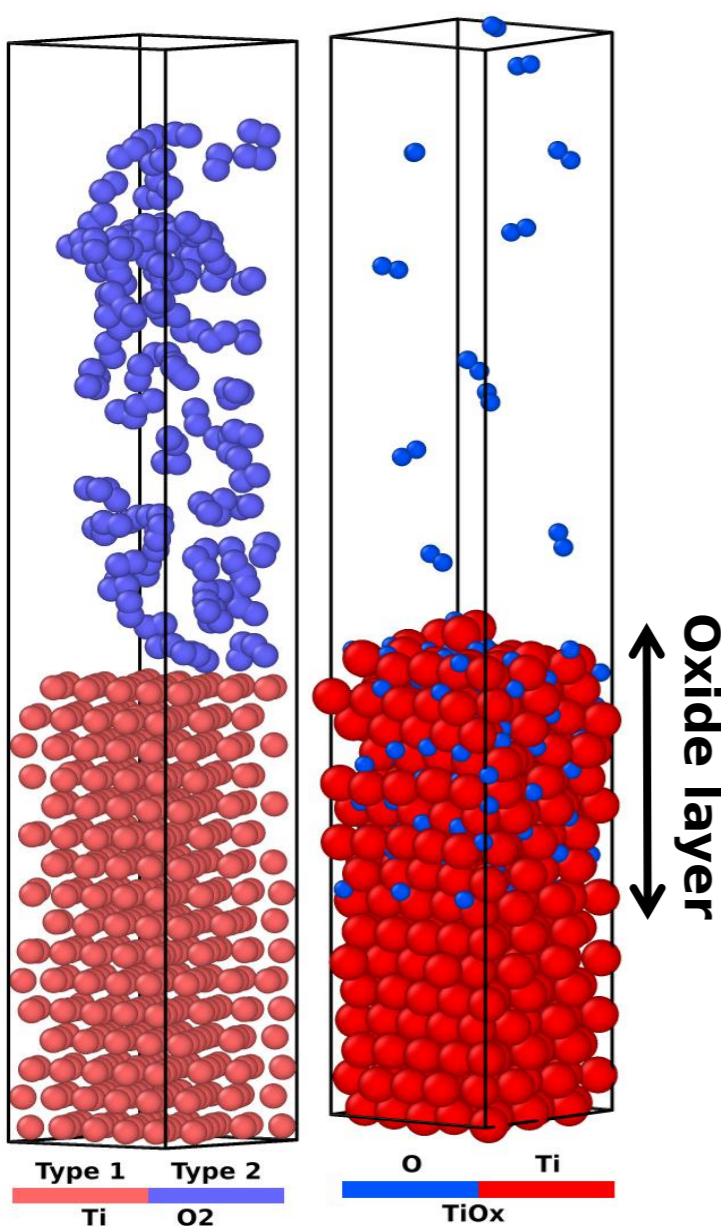


Fig. 2. Oxidation process of Ti

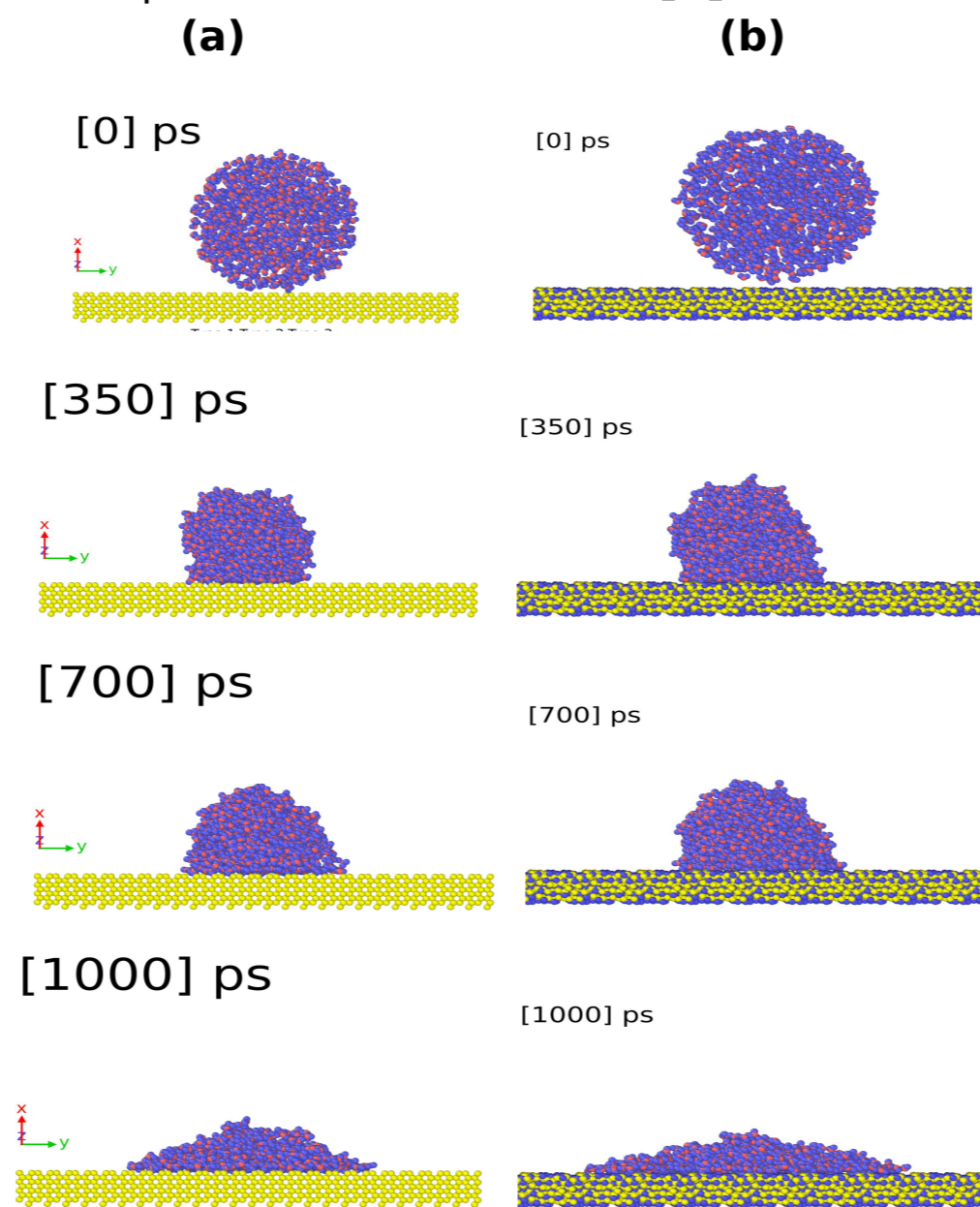


Fig. 3. Wettability of (a)Ti and (b) TiOx

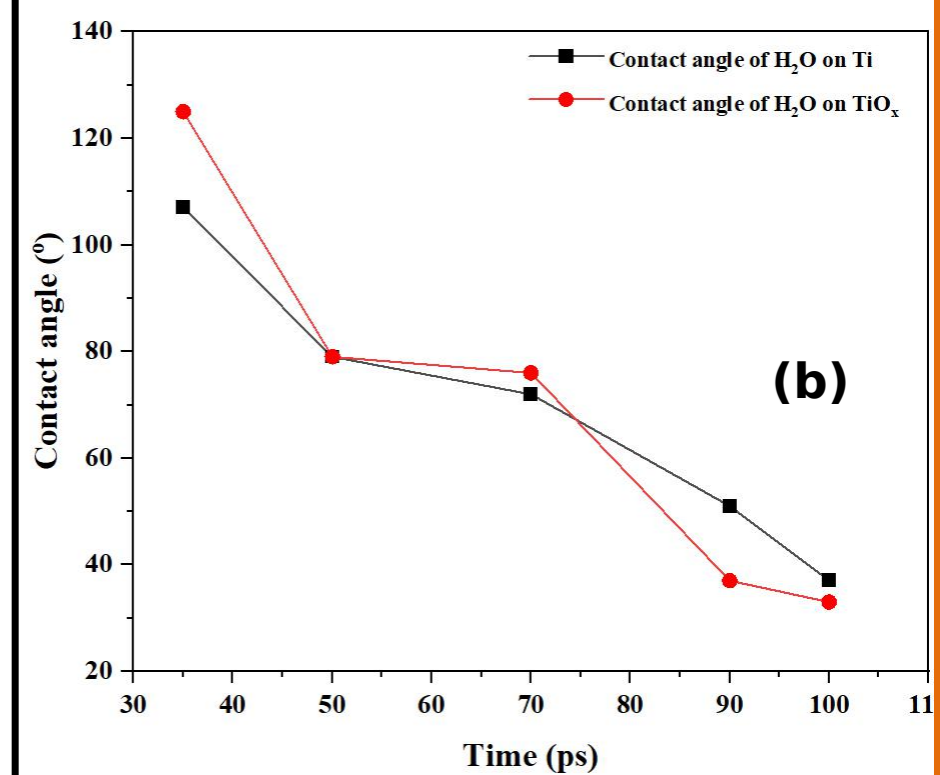
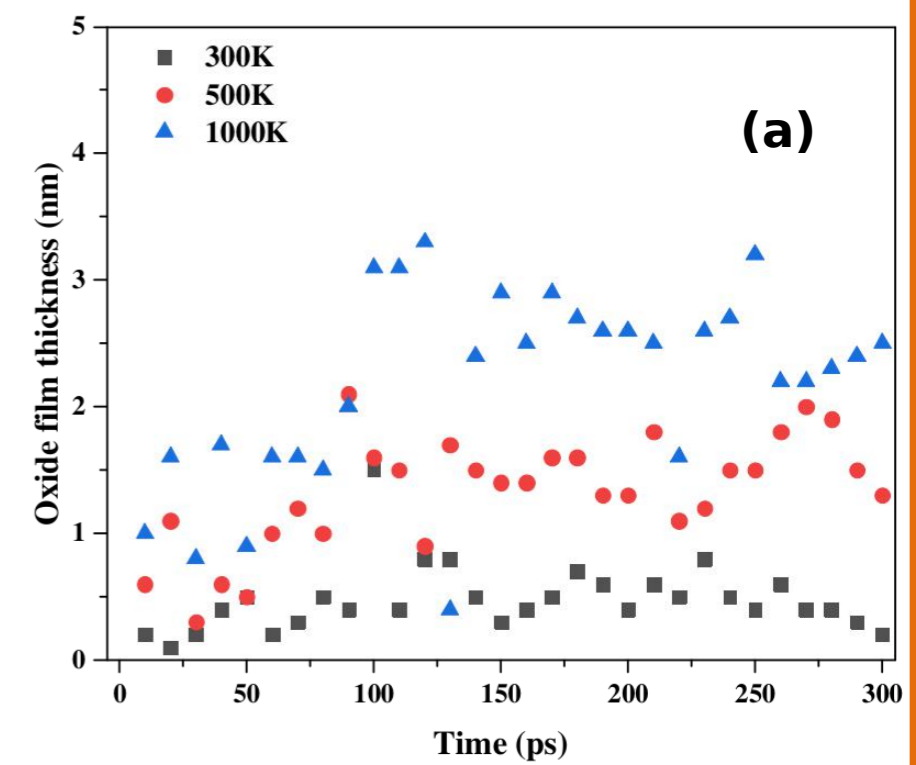


Fig. 4(a). Oxide film thickness (b). Wettability of Ti and TiOx

## 5.0 Conclusion

- The surface chemistry of laser-treated surfaces plays a pivotal role in how the wettability changes over time. Our calculations shed light on the early oxidation process of titanium (Ti) and its impact on the wetting properties of such surfaces.
- Experimental observations align with our findings, indicating that the presence of oxide on the surface diminishes the hydrophobic behavior of droplets.

### References

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