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. In particular, micro- and nanotextured surfaces find numerous applications in virus and bacterial repulsion, including the osseointergration process in biomedical implants. Laser treatment is one of the most efficient tools for surface texturing opening numerous possibilities of the control over the produced reliefs. 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. To gain further insights into these effects, we performed reactive molecular dynamics (RMD) simulations with hybrid TTM-MD to understand the effect of early oxidation on wettability of laser-treated titanium (Ti) (fig. 1).

1.1 Study Outlook

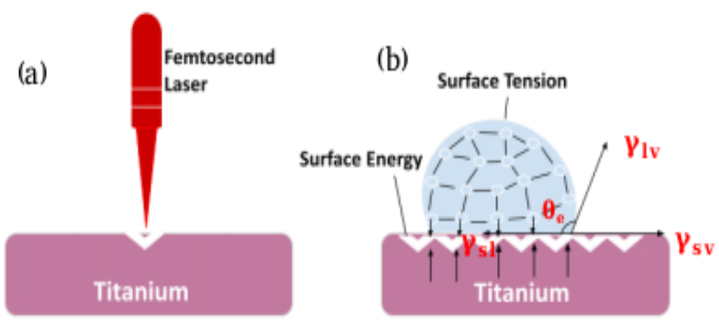

Fig 1. wettability of laser-treated titanium

2.1 TTM-MD and Reaxff

We used hybrid approach that combines traditional molecular dynamics (MD) with a two-temperature and molecular dynamics (TTM-MD) model for the interaction between ultrafast laser and Ti. The modeling consisted of two parts: [1] MD, which describe the behavior of the lattice subsystem, and the continuum part, classical TTM, which accounted for processes in the electron subsystem.

To accurately capture bond breaking and formation, we employed the reactive force (reaxff) field as described by the reaxff equation in Section 2.0.

2.0 Computational Details

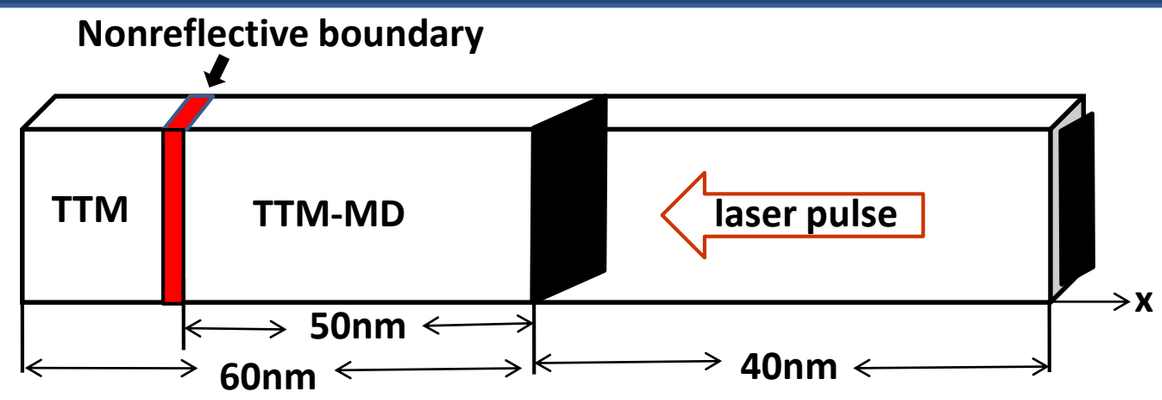

Fig 2. wettability of laser-treated titanium

MD-TTM Model

$$① \quad C_e(T_e)\frac{\partial T_e}{\partial t} = \nabla\cdot[K_e(T_e,T_i)\nabla T_e] - G(T_e)(T_e - T_i) + S(\vec{r},t)$$

$$② \quad C_i(T_i)\frac{\partial T_i}{\partial t} = \nabla\cdot[K_i(T_i)\nabla T_i] + G(T_e)(T_e - T_i)$$ — TTM

$$③ \quad m_i d^2\vec{r}_i/dt^2 = \vec{F}_i + \xi m_i \vec{v}_i^{th}, \quad T_i^{cell} = \sum_{cell} m_i\left(v_i^{th}\right)^2/(3k_B N_{cell})$$ — MD

REAXFF Potential

$$\mathrm{BO}'_{ij} = \mathrm{BO}^{\sigma}_{ij} + \mathrm{BO}^{\pi}_{ij} + \mathrm{BO}^{\pi\pi}_{ij}$$
$$= \exp\left[p_{\mathrm{bo},1}\left(\frac{r^{\sigma}_{ij}}{r_o}\right)^{p_{\mathrm{bo},2}}\right] + \exp\left[p_{\mathrm{bo},3}\left(\frac{r^{\pi}_{ij}}{r_o}\right)^{p_{\mathrm{bo},4}}\right]$$
$$+ \exp\left[p_{\mathrm{bo},5}\left(\frac{r^{\pi\pi}_{ij}}{r_o}\right)^{p_{\mathrm{bo},6}}\right],$$

Table 1: Model Validation

	LAMMPS	Experiment
a (hcp) (Å)	2.909	2.951[a]
c/a (hcp) (Å)	1.588	1.588[a]
Ecoh (kcal/mol)	−115.04	−115.00[b]

3.0 Results

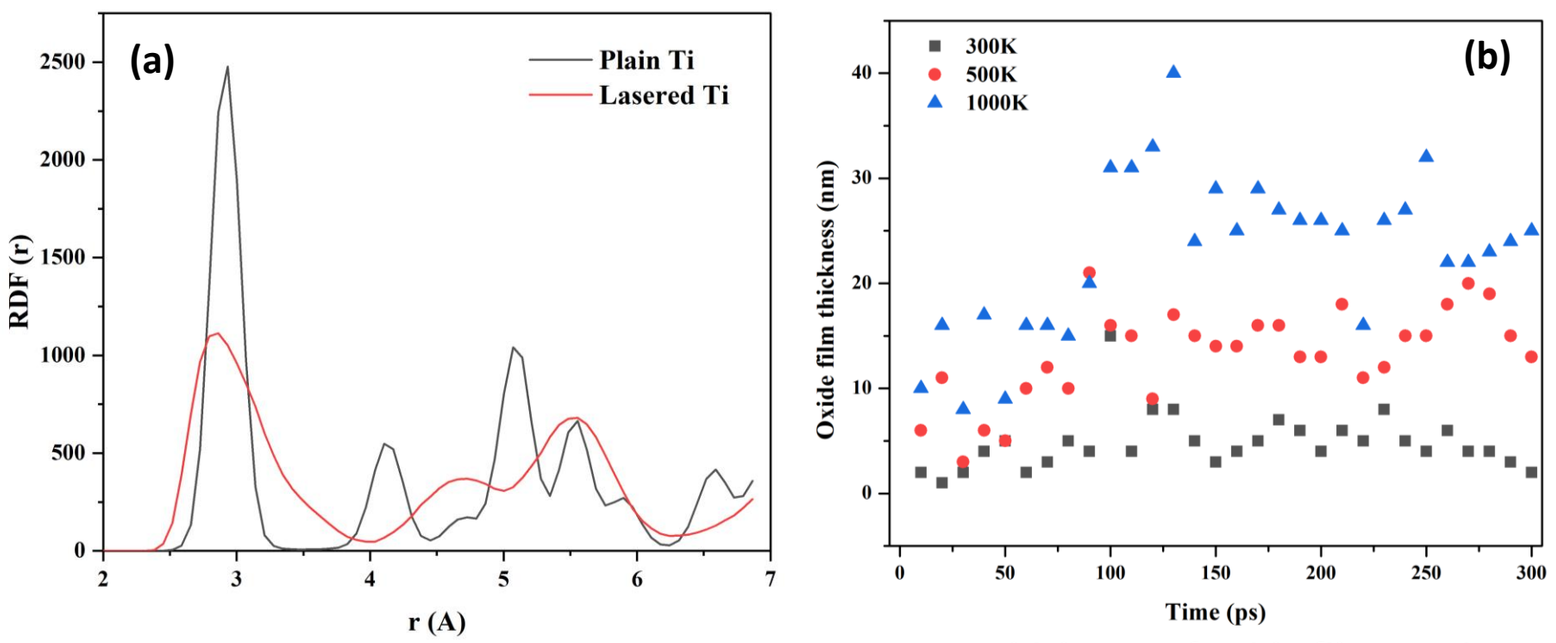

Fig. 3 (a) RDF of Ti (with and without laser) and (b) Thickness of oxide film on Ti

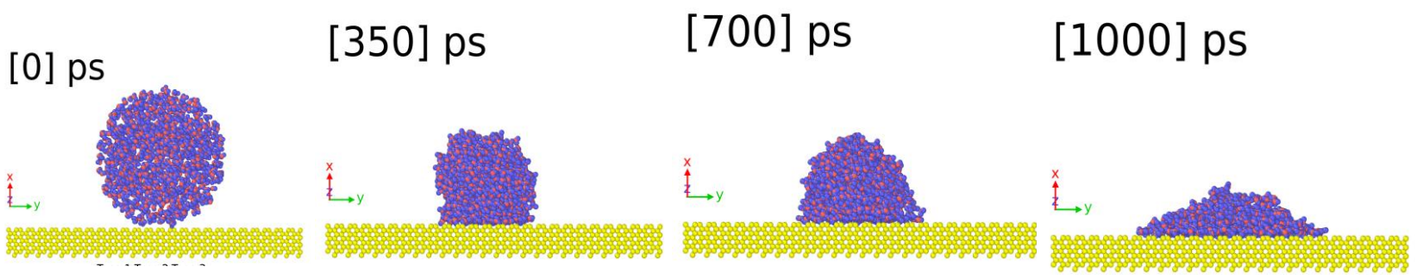

Fig. 4. Wettability of Ti (without laser)

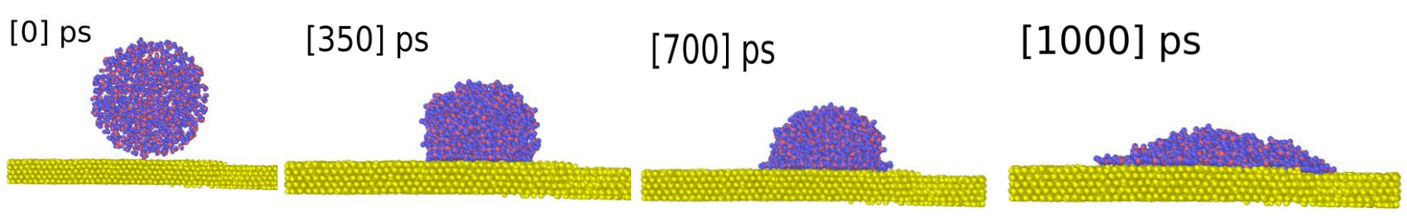

Fig. 5 Wettability of Ti (with laser)

4.0 Discussion

The obtained results show that the femtosecond laser significantly change the structure of Ti as shown in fig.3a. Interestingly, when O2 is been introduced on Ti, the oxide thickness increases with time (Fig. 3b). Hence, the TiOx 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 TiOx layer and a decrease in O2 diffusion, which thus, affects the wettability of Ti (fig4 and 5).

5.0 Conclusion

The wettabbility of Ti show that the presence of oxide makes the droplet behavior less hydrophobic in agreement with experiments. Because oxide layer thickness rises with time, the contact angle drops down with time which is more in lasered Ti. 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 correlate.

References

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