Surface Functionalization of Polyurethane Towards Prevention of Biomaterials-Centered Infections: Combined Experimental and Molecular Dynamics Simulations Approach

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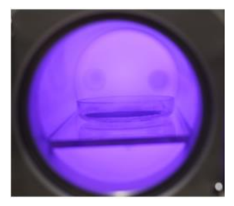
Abstract

Although commonly used, polyurethane biomaterials still need improvement in terms of their affinity to microorganisms [1]. Biomaterial surfaces can be contaminated during surgery, mostly by bacteria strains that are harmless for healthy people e.g., species of the genera Staphylococcus and Pseudomonas. Biomaterial-cantered infection (BCI) may lead to secondary complications i.e. amputations, morbidity, and even mortality. The most important aspect that has to be taken into consideration while designing new biomaterials surfaces is the competition for the surface between eukaryotic cells and microorganisms, which is called 'race for the surface'. The outcome of this contest is critical for the patient since if bacteria attach to the medical device, they colonize it and produce biofilm. Therefore, the biomaterial surface has to be adequately prepared to increase biocompatibility and at the same time, limit the risk of bacterial infection. The most common functionalization to increase the surface biocompatibility of polymeric materials is the formation of oxygen-containing groups by plasma modification. Such treatment indeed increases biocompatibility, but at the same time significantly higher bacteria affinity to such surfaces is observed [2]. The mechanism of this effect remains unsolved so far, mostly because the studies are performed in the microscale. The study aimed to use combined in vitro (AFM, XPS, SIMS, biological tests) and in silico (MD) experiments and provide the basis for a better understanding of the complex interplay between biomaterial surface properties and early steps of BCI.

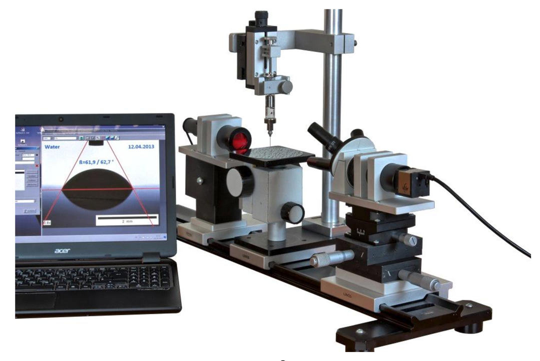
Materials and Methods



oxygen plasma treatment

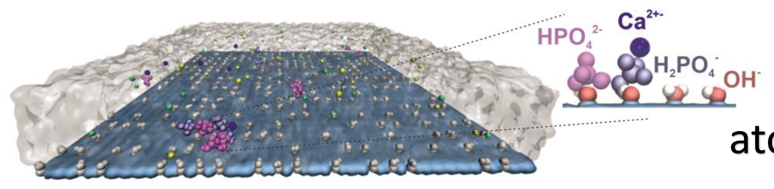
SEM

XRF



contact angle measurements

AFM



atomistic MD simulations

Results and Discussion

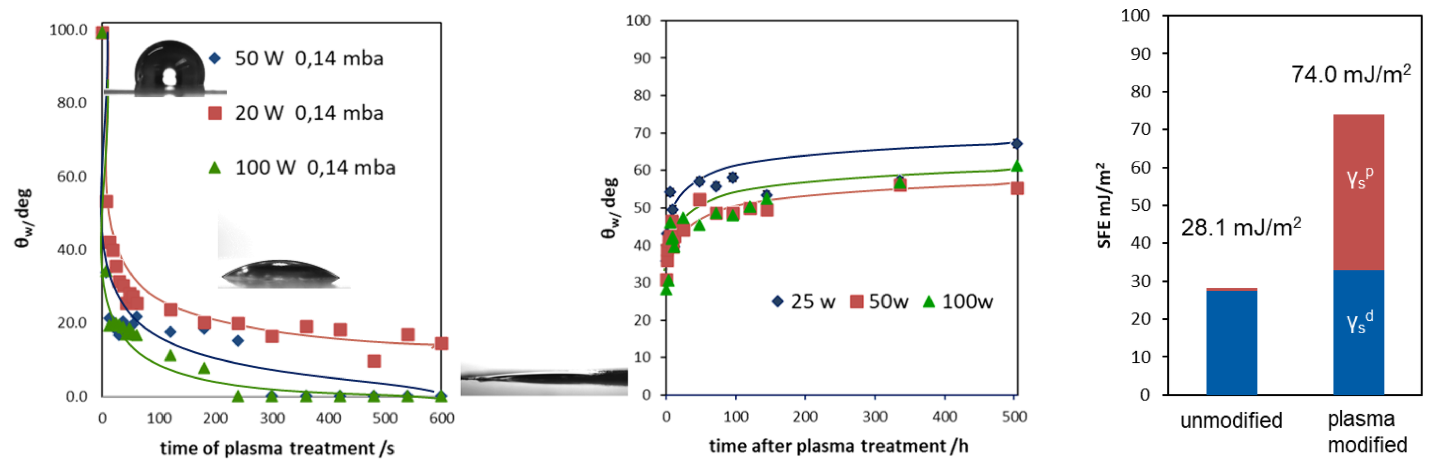


Fig.1 Contact angle values and SFE obtained for unmodified and oxygen plasma modified polyurethane.

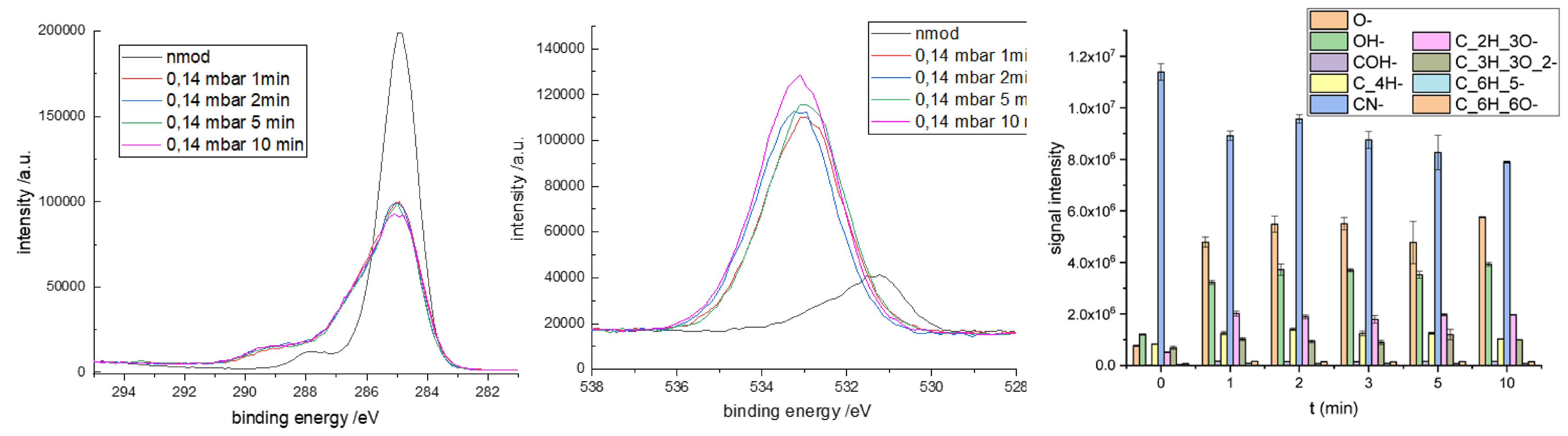


Fig.2 XPS and SIMS spectra for unmodified (nmod) and oxygen-plasma modified polyurethane.

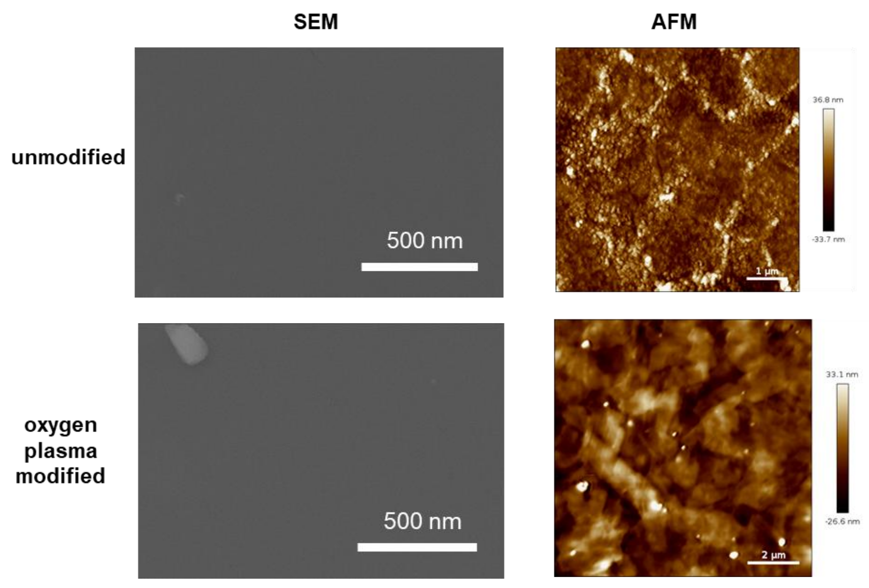


Fig.3 Surface topografy of unmodified and oxygen-plasma modified polyurethane.

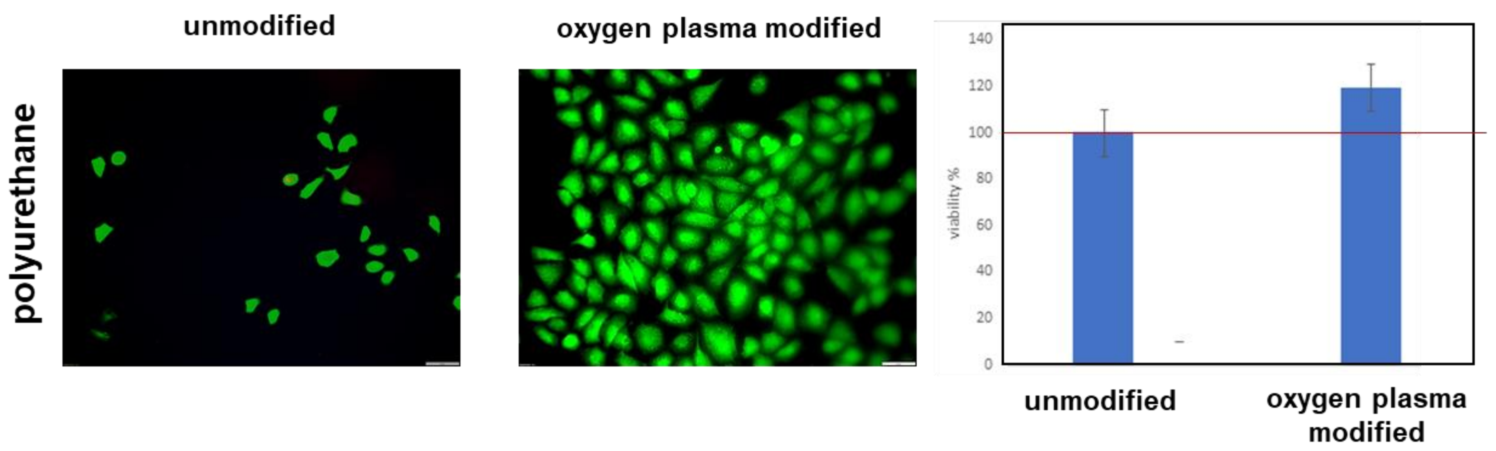


Fig.4 FDA/PI staining of A549 human lung adenocarcinoma on polyurethane surfaces, accompanied by viability results.

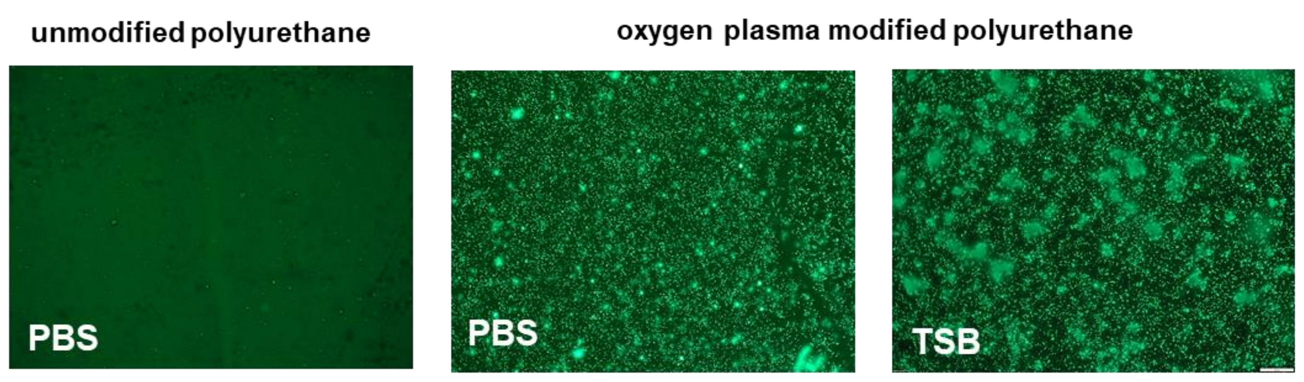


Fig.5 LIVE/DEAD staining of S. aureus on poyurethane surfaces

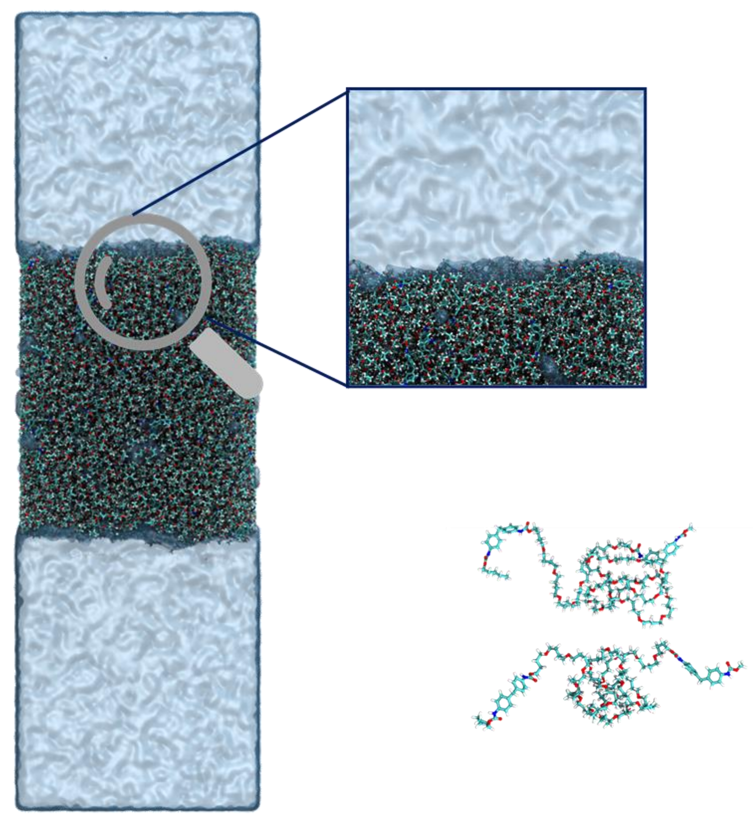
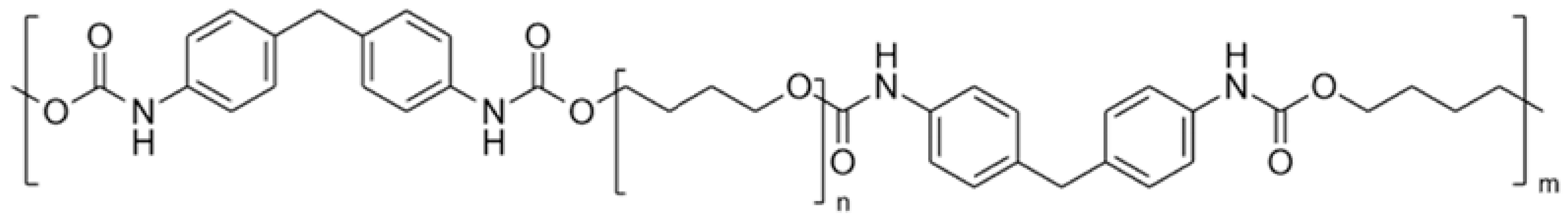


Fig.6 MD simulation boxof poyurethane/water interface



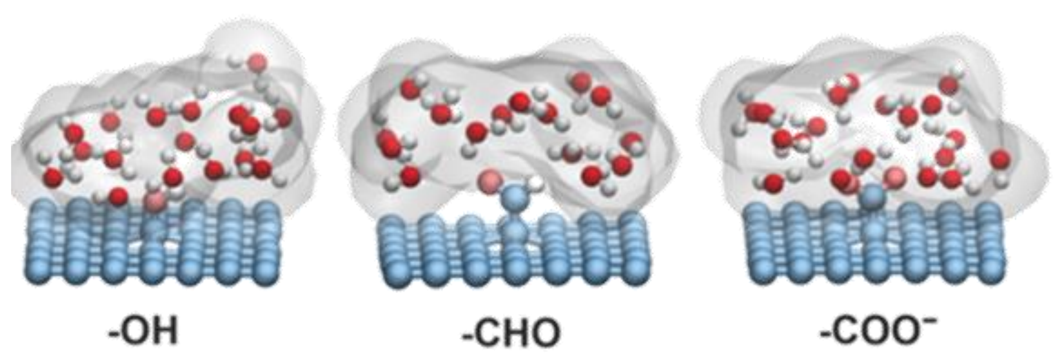


Fig.7 Representative fragments of decorated polymeric surfaces showing interaction of various surface groups with water molecules. Gray shadowing based on isovalues of water density illustrates the hydrophilic properties of the surfaces.

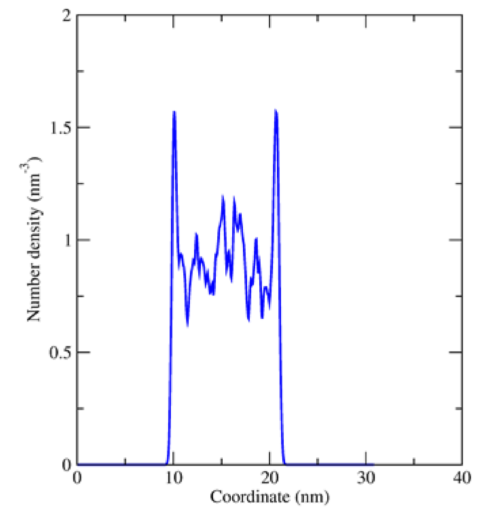


Fig.8 Nitrogen distribution

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Conclusions

- Novel strategies to prevent BCI are needed (urgent!)
- Plasma is an effective tool to functionalize polymeric surfaces without damaging their bulk
- Molecular-level in silico apprach supported by experimental results can be successfully used for biointerface design and fabrication
- The results are promising in terms of controllable tuning and functionalization of implantable polymeric materials