Simulations reveal role of calcium in titanium implant acceptance

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Titanium-based materials are widely used in medical implant technology. Coating the surface of titanium materials with biologically active molecules has recently shown promise to improve how cells adhere to implants and promote tissue regeneration. The mechanisms behind how peptides stick to titanium, however, are not fully understood.

Researchers at Deakin University in Australia found how calcium ions present at the interface between titanium oxide and tissues affect how well peptides bind to the metal. The team reports their findings in a special issue of *Biointerphases*, that is highlighting women in the field of biointerface science. Using recently developed tools in molecular dynamics simulations, the group's findings provide an early understanding in how one day we might use salt's composition to finely tune the reactions between titanium implants and the body.

"This work contributes to a long-running and ongoing effort to identify systematic improvements for load-bearing implant materials," said Tiffany Walsh, an author on the paper. "The binding behaviors we have identified for these peptides in the presence of ions might guide others in the design of new implant coatings."

It is believed that coating titanium surfaces with biomolecules to adhere to host tissues is aided by nearby inorganic ions in the body. Because of their higher positive charge and role in cell signaling, calcium ions are suspected to be particularly helpful.

To tackle these questions, Walsh and her colleagues created a computer model of the oxidized surface of titanium. The group simulated two titanium-binding peptides, Ti-1 and Ti-2, in solutions of calcium chloride and sodium chloride using molecular dynamics simulations. This computation approach approximates and models the interactions between the numerous molecules in a system. In their model, they relied on an advanced technique called replica exchange with solute tempering that accelerates the exploration of the peptide structures.

The group discovered that positively charged calcium ions helped Ti-1 adhere to the titanium surface by acting as a connector between the negatively charged titanium oxide and asparagine, a residue within the Ti-1 peptide. This process then leads to other residues pinning directly to the titanium oxide surface. For Ti-2, however, calcium ions were found to limit access to the surface.

The data from their simulations point to improved principles for designing peptides with tunable a?nity to titanium application. Walsh said she expects that their findings will lead to exploring the titanium-tissue interface further, including molecules with one binding domain for titanium and one for biomolecules.

"Titanium is a common implant material, and our comprehension of how to beneficially modulate the interaction between titanium and living tissue, while very advanced, still has a lot to go," Walsh said. "We want to contribute to this ongoing effort."

More information: "Effect of calcium ions on peptide adsorption at the aqueous rutile titania (110) interface," *Biointerphases*, DOI: 10.1063/1.5046531

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