Exploring the basic mechanisms of bacterial contact formation and breaking: Combining AFM force spectroscopy & MC simulations

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Combining single bacterial probe force spectroscopy [1] with Monte Carlo (MC) simulations [2], a multitude of details on the bacterial adhesion process is gained [3,4]. As bacterial probes, we use cocci, e.g. *Staphylococcus aureus*. Already the form of the force/distance curve (FDC) upon approach of the bacterium to the solid is characteristic for the type of binding between the bacterial cell and a specific surface. On hydrophobic surfaces, the FDCs exhibit a pronounced snap-to-contact at a distance of ~50 nm from the surface, a process that can be eliminated by cutting or crosslinking proteinaceous components of the cell wall [2]. To mimic the experimental FDCs, MC simulations need to take ten thousands of macromolecules (simulated as elastic springs with a distribution of spring constants) into account to make contact via hydrophobic interactions to the surface. However, on hydrophilic surfaces, experimental FDCs display no snap-to-contact, and only a few tens of elastic springs are needed in the MC simulations to mimic the curves. The force to remove the bacterium from the hydrophilic surface is an order of magnitude smaller than on hydrophobic surfaces, where the hydrophobic effect plays the main role. Experimental determinations of the size of the contact zone of the bacterial cell suggest that adhesive force and contact area are not correlated [4]. Rather, differences in cell wall macromolecule composition determine the adhesive behavior.

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