411g Quenching of Growth of Asa Crystal Surfaces by Adsorption of Various Surfactant Molecules Using Molecular Dynamics Simulations

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To exploit properties of nanoparticles, it is essential to effectively control their size. We investigate properties of several non-ionic surfactant molecules that quench crystal growth using both experimental and computational techniques. We perform molecular dynamics simulations on the adsorption of five model surfactant molecules based on the structure of Brij 78, Brij 700, Poloxamer 188, Poloxamer 338, Poloxamer 407, and Tyloxapol, onto the three major surfaces of the aspirin crystal, i.e. (100), (001) and (010) in the presence of either a polar solvent (ethanol) or a non-polar solvent (hexane). Our results indicate that depending on the type of solvent considered and degree of polarity of the surfactant, the adsorption of surfactant molecules on the surface of the crystal is in some cases surface specific. Hydrogen bond and van der Waals interactions play major roles in the affinity of the surfactant on the surface of the crystal, and in turn in the surfactant quenching effect. For the Poloxamer series, as we decrease the degree of hydrophilicity of the model surfactants by changing the number of block units (i.e. EOxPO(8-2x)EOx (EO=ethylene oxide; PO=propylene oxide; x = 0,1,3, and 4)), we find that the binding energy of the surfactant segment with the aspirin surface increases regardless of the solvent environment, and it is not surface specific. These types of surfactants effectively quench aspirin crystal growth and in most cases do not cause morphology modification. These theoretical findings are inline with the results from our recrystallization experiments, and will be the topic of this presentation.