Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Molecular Dynamics Simulation of Hybridization Kinetics of Surface-Grafted DNA NAIDA LACEVIC, Lawrence Livermore National Laboratory, ARUP CHAKRABORTY, Dept. of Chemical Engineering UC Berkeley — Increasing interest in development of biosensors results in a need to understand all levels of design and operation of these devices. We focus on a DNA biosensor that is based on molecular recognition between nucleic acids and the subsequent hybridization process. In order to effectively design such a biosensor, it is necessary to understand the effects of grafting density and sequence mismatch on hybridization efficiency. These are of direct relevance to device performance as hybridization efficiency and density determine the signal strength. We use molecular dynamics (MD) simulations to elucidate effects of grafting density on hybridization efficiency and hybridization density as well as the effects of sequence mismatches on hybridization in surface-grafted DNA. We have developed a "minimal" coarse-grained model of DNA suitable for long timescale molecular dynamics simulation. We have calculated the hybridization efficiency and conformational order parameter $Q_{\alpha\beta}$(**r, r'**) between target and probe DNA from MD trajectories. We find that the hybridization efficiency decreases with increase of grafting density, as seen in experiments. We also find that target DNA binding to multiple probes is a dominant effect at higher grafting densities and represents a major obstacle to efficient hybridization efficiency. We show that the width and amplitude of $Q_{\alpha\beta}$(**r, r'**) are sensitive to the grafting density and number mismatches on the target, respectively.

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Date submitted: 03 Dec 2004 Electronic form version 1.4