MULTISCALE SIMULATION OF LIQUID CRYSTALS

Applications in the modeling of LC-based biosensors

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Abstract Nematic liquid crystals are characterized by the occurrence of disclination lines, topological defects where the average molecular orientation changes abruptly. Recent experiments have shown that, in addition to their application in displays, liquid crystals permit the detection of ligand-receptor binding by optical amplification. The optimal design of LC-based biosensors requires an understanding of the effects of the presence of biomolecules on the structure and dynamics of nematic liquid crystals. We present a multiscale approach that combines molecular simulations and mesoscale modeling: Monte Carlo simulations are used to study the interactions of dilute colloidal particles, as well as the structure of topological defects; these results compare satisfactorily with the corresponding theoretical calculations at the mesoscale level. The mesoscale modeling of a multi-particle sensor shows that adsorbed biomolecules modify the relaxation dynamics in the device: at low surface-coverage densities, the equilibrium structure is characterized by a slightly perturbed uniform nematic order; at a critical density, the dynamics exhibits a slowdown at late stages, characteristic of the inability of the nematic to achieve a uniform order. These results are compared with experimental observations of the nematic response in biosensors.

Introduction

Consider a device capable of transducing and amplifying the binding of proteins or viruses at surfaces into optical signatures that could be easily read with the naked eye. In order to do so, the device would have to bridge length scales over four orders of magnitude: from the size of a protein (10nm) to patterns large enough for the eye to see (0.1mm).
Such devices have in fact been in existence for half a decade. The basic elements are (see Fig.) a thin film of a liquid crystal (LC) sandwiched between ligand-conjugated self assembled monolayers (SAMs), supported by semitransparent gold films on glass substrates [1, 2].

Figure 1. A schematic view of a liquid crystal-based biosensor: a thin film of a nematic liquid crystal is confined between parallel walls. The walls are assembled using self-assembled monolayers (SAMs) formed from ligand-conjugated thiols and alkanethiols on semitransparent gold films supported on a thin layer of titanium supported by glass. (For clarity, the titanium and glass layers are not shown.)

The principle of operation of this kind of biosensors relies on several characteristic properties of LCs [1]: first, they exhibit long range orientational order, which means that LCs can report events and orientations to regions that are macroscopic length scales away (e.g. 0.1 mm). Second, because LCs are fluids, the changes induced by binding events at the surface can propagate throughout the medium relatively rapidly. And finally, the optical anisotropy caused by the local preferred orientation of the mesogens is easily transduced into an optical signal that can be read with ambient light.

The anchoring behavior of the LC at the substrates is controlled by the surface chemistry [3] or topography [4] at the nanometric scale, so that in the absence of binding events the orientation of the mesogens is uniform throughout the sensor. But when ligand bounds to the receptors, the preferred orientation at the surface is no longer uniform. This is translated into an optical image that shows a proliferation of multidomains and topological defects as the concentration of ligand is increased [2].

However, the design and optimization of liquid crystal-based biosensors would benefit from a fundamental understanding of the structure and dynamics of the domains and defects that are present in the de-