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Markov decision process based time-varying optimal control for colloidal self-assembly

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Abstract: Crystals made of periodically well-ordered nano- and/or micro-scale elements can interact with light to give novel properties. These perfect crystals have applications in a wide range of areas. For example, invisibility cloaks that reroute light transmission make objects disappear. However, manufacturing such perfect crystals still remains challenging. Here, we propose a low-dimensional Markov decision process based dynamic programming framework to optimally control a colloidal self-assembly process for perfect crystal fabrication. Based on the simulation results, we demonstrate that an open-loop control policy identified with the proposed framework is able to reduce the defective assemblies from 46% of uncontrolled to 8% of controlled production. Moreover, when feedback is available, a closed-loop optimal finite-horizon control policy can further reduce the defective assemblies down to 5% out of 100 independent simulation runs.

Keywords: optimal control, feedback control, open-loop control, dynamic programming, stochastic control.

1. INTRODUCTION

Crystals composed of periodically well-ordered small elements possess the ability to interact with light at specific wavelengths. Micro-scale particles suspended in solution are called colloids, and assemblies made of colloids can be ordered at the same length scale as light wavelength. A recent study by Ni reported the feasibility of making an ultrathin skin cloak out of nanoantenna that is able to reroute light and render objects invisible (Ni et al. (2015)). Other applications include: adaptive optics (Holtz and Asher (1997)), reconfigurable circuit elements (Yang et al. (2009)), semiconductors (Velev and Lenhoff (2000)) and so on. Despite the attractive applications, manufacturing perfectly ordered colloidal assemblies over larger scales is still challenging. Currently available manufacturing methods can be generally defined into two categories: *top-down* and *bottom-up* methods (Biswas et al. (2012)). Top-down fabrication such as lithography, is achieved largely by patterning features. It starts from larger dimensions and reduces to the required values (Gates et al. (2005)). On the other hand, bottom-up fabrication, like self-assembly, builds up assemblies from smaller components (Ariga et al. (2008)).

Top-down approach has shown success as reported in Biswas et al. (2012) and its references. However, bottom-up approach provides a more promising fabrication for large quantities with less waste and better quality control (Biswas et al. (2012)). Indeed, time-varying actuator setting in external field mediated assembly processes has already shown its effectiveness. For example, Swan et al. (2014) demonstrated the use of a time varying magnetic field for a large assembly of ordered paramagnetic colloidal particles. In a magnetic field mediated self-assembly system, particles are driven together when the field is turned on, and are allowed to diffuse for rearrangement when the field is turned off. Swan illustrated that by periodically switching between a high and a low field strength at appropriate frequency (i.e. toggling), they were able to create a condensed crystalline assembly of polystyrene latex particles (Swan et al. (2014)). The idea of designing such an annealing scheme makes physical sense, with external forces used to accelerate the assembly and turned off when disorder is formed.

However, particles at micro-scales are subjected to Brownian motion and possess different dynamics each time. Therefore, none of the open-loop control schemes could provide an optimal assembly strategy every time. On the other hand, feedback control with real-time sensing using optical microscopy and image analysis, can help to avoid or correct for defects by designing the optimal actuator settings with instant information.

In past work, we built a low-order model based on two order parameters for an electric field mediated colloidal self-assembly process. In this system, strength of interactions between particle and field, as well as particle and particle, was controlled by changing the amplitude of the input voltage. A detailed particle-scale Brownian dynam-

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ics simulation was used to generate samples for construction of a Markov state model (Bowman et al. (2014)). The Markov state model was then used to calculate the optimal control policy (i.e. input voltage trajectory) using dynamic programming, via a Markov decision process framework (Puterman (2005)). With the objective to maximize the global crystallinity ψ_6, 98 out of 100 independent experiments (i.e. a 98% yield) produced a perfect assembly (i.e. assembly with a higher than 0.96 ψ_6 value) with the control policy compared to a 60% yield under a constant high input (Tang et al. (2016)).

The closed-loop policy calculated in the previous work was time-independent, here we calculate a time-dependent closed-loop optimal policy, using a finite-time formulation of the Markov decision process. The objective is now to maximize global crystallinity at a pre-specified terminal time. The incorporation of time-dependence brings in more flexibility by yielding different control policies at different updating time point. It also adds physical insight into the optimality of switching between a high and low input level (Swan et al. (2014)). In fact, in our past work with a *time-independent* policy, we also observed similar switching patterns, due to the system transitioning between different regions of the state space. In addition to closed-loop policies, the Markov state model are also used to calculate an optimal open-loop policy to maximize expected final crystallinity. This further allows us to understand the optimality of simple toggling schemes.

2. COLLOIDAL ASSEMBLY SYSTEM

2.1 Experimental Setup

In this study, we focused on a SiO_2 colloidal particle assembly process (Tang et al. (2016),Juárez et al. (2012)). In this system, about 300 SiO_2 particles with a radius of 1.5 μm are suspended in deionized water in a container made of glass microscope cover slips (50 mm x 24 mm x 150 μm). Four separate, tunable 1 MHz AC electrode tips are attached to the edge of the container to generate a non-homogeneous electric field. The system is monitored in real time using a microscope.

In an AC electric field mediated colloidal self-assembly system, colloidal particles become induced dipoles when the field is turned on. The interaction between the electric field and the particles, together with the particle-particle interactions, provides the driving force for the crystallization. A detailed study of the electric-field mediated assembly mechanism is presented by Juárez and Bevan (2009). In order to make a direct comparison to the toggling scheme, only two input levels are considered here: $\lambda = 0.2$ and $\lambda = 19.7$, where λ is a dimensionless representation of voltage, indicating the strength of the driving force (Tang et al. (2016)).

Fig. 1 shows the experimental setup (Fig. 1a), top-view zoomed in to the assembly system (Fig. 1b), with electrode distance as 96 μm, particle configurations under the low input $\lambda = 0.2$ (Fig. 1c), and the high input $\lambda = 19.7$ (Fig. 1d,e,f). The local hexagonal order C_6 is colored in blue, and the global hexagonal order ψ_6 colored in red. Index 6 associated with the order parameters indicates the maximum number of neighboring particles of each particle

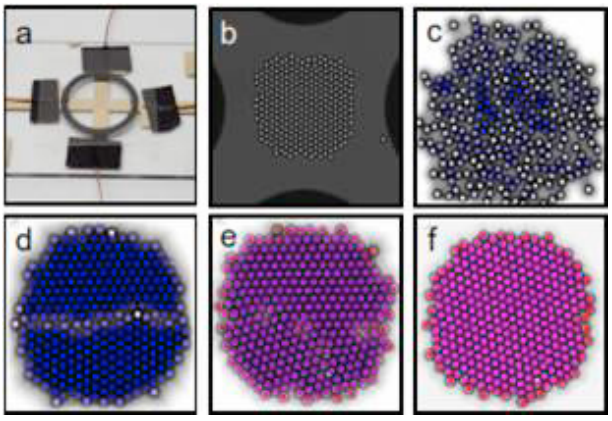

Fig. 1. Experimental setup and colloidal self-assembly process: (a) colloids container with four electrodes attached; (b) top view of colloidal assembly process under microscopy; (c) colloidal system in fluid state under the lowest input level; (d) grain boundary under the highest input level; (e) defective under the highest input level; (f) perfect crystalline state under the highest input level. With color blue indicating the local hexagonal order C_6, and red indicating the global hexagonal order ψ_6 (Tang et al. (2016)).

in a 2-dimensional plane. The system exhibits a fluid state at $\lambda = 0.2$ while reaching a perfect crystal at $\lambda = 19.7$ (Fig. 1f). However, due to the strong attractive force, grain boundaries and defective structures also tend to form under the high input (Fig. 1d,e). In this study, we focus on removing the grain boundaries from the 2-dimensional assemblies.

2.2 Brownian Dynamics (BD) Simulation and Order Parameters

Building an optimal control policy for a stochastic process requires a thorough understanding of the system dynamics. With an accurate model, it is then possible to effectively study the dynamics over a wide range of repetitions and under extreme conditions. A Brownian dynamics simulation was built and validated against experiments to simulate the system dynamics (Edwards et al. (2013)). The Cartesian coordinates of each particle, together with its velocity, are used as the input for the simulation; therefore it is a $4N$-dimensional simulation model, where N is the number of particles. The BD simulation provides an accurate prediction of the system by tracking the individual particle positions. The detailed background on the Brownian dynamics simulation is given in Edwards et al. (2014).

However, keeping track of all the particle coordinates makes the simulation a time-consuming process. More importantly, using the entire Cartesian coordinates as a state description hinders the calculation of a control policy due to the high dimensionality. Instead, it is often useful to calculate a reduced set of coordinates, which captures the overall system features of interest. This would introduce errors to the reduced-order model, but it makes the state classification feasible and the control approach tractable. The dimensionality reduction can be accomplished using physical intuition, computer algorithms, or a combination