Quantifying the Response of Diverse Nanoparticles Towards Laser-Induced Thermoelectric Field to Enhance Applications in Nanorobotics

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Abstract: Thermoelectric field around colloidal nanoparticles in laser-induced, spatially varying thermal gradients is theoretically derived. Experimental validation is also presented for diverse scenarios of laser-induced trapping, rotation and pulling of polystyrene, Janus and silicon nanoparticles, respectively.

1. Introduction:

Opto-thermoelectric nanotweezers [1] were recently proposed to overcome the notable limitations of optical tweezers such as high laser power requirement and limited diversity in materials and the size of the nanoparticles. This technique uses the differential movement of cations and anions under laser-induced thermal gradient to create a thermoelectric field pointed towards the laser spot, enabling the trapping of positively charged particles at the laser center. The thermal gradient is created through the heating of a plasmonic substrate which has high photon-phonon conversion efficiency resulting in high temperatures for laser powers much lower than optical tweezers. Although this technique has been excellently employed to trap and manipulate metallic, biological and dielectric particles [2], the underlying physics is not fully understood due to the complexity of multiple force fields such as optical, osmotic and thermoelectric forces interacting constructively. Also, the theory on thermoelectricity in colloidal solutions has been developed with a major assumption of a constant temperature gradient around the nanoparticles, which fails to explain several practical phenomena observed during the particles' interaction with lasers, thereby limiting their implementation in applications [3]. Therefore, improvisation in thermoelectric field formulation is essential for of advancement of applications in nanorobotic studies.

2. Theory, Results and Discussion:

Herein, we proposed to bridge this theoretical deficit by numerically evaluating the thermoelectric forces and torques of nanoparticles by considering the spatial-variation of the field around the particle [4]. We prove that the implementation of a constant temperature gradient across a particle would also result in a distortion of the temperature gradient around the particle due to discontinuity in the thermal conductivity at the interface (Fig. 1a). The resultant temperature gradient results in an ionic distribution which results in a thermoelectric field due to the electrolyte (in this case – a monovalent surfactant CTAC), formulated as

$$\boldsymbol{E_T} = \frac{k_B T \boldsymbol{\nabla T}}{e} \frac{\left[\frac{Z_1 S_{T_1}}{N_{agg}} + S_{T_2}\right]}{1 - \frac{Z_1 S_{T_1} T}{N_{agg}}} = SC\nabla T \tag{1}$$

where $\boldsymbol{E_T}$ is the thermoelectric field, k_B, e, T and ∇T are Boltzmann constant, electron charge, temperature and its gradient respectively. S_{T_1} and S_{T_2} are the Soret coefficients of surfactant micelle and chlorine ion, while N_{agg}, Z_1 and Z_2 indicate the aggregation number, valency of CTAC micelle and valency of chlorine ion respectively.

Physical manifestation of charge separation is not observed in simulations due to low temperature gradients (10 K/μm) utilized in this work. The parallel component of the thermoelectric field (Fig. 1b) interacts with the charge on the particle while the perpendicular component of the field is attenuated due to double layer screening (Fig. 1c), indicating that the response of the particle towards the temperature gradient is only due to the drag component of thermoelectric field.

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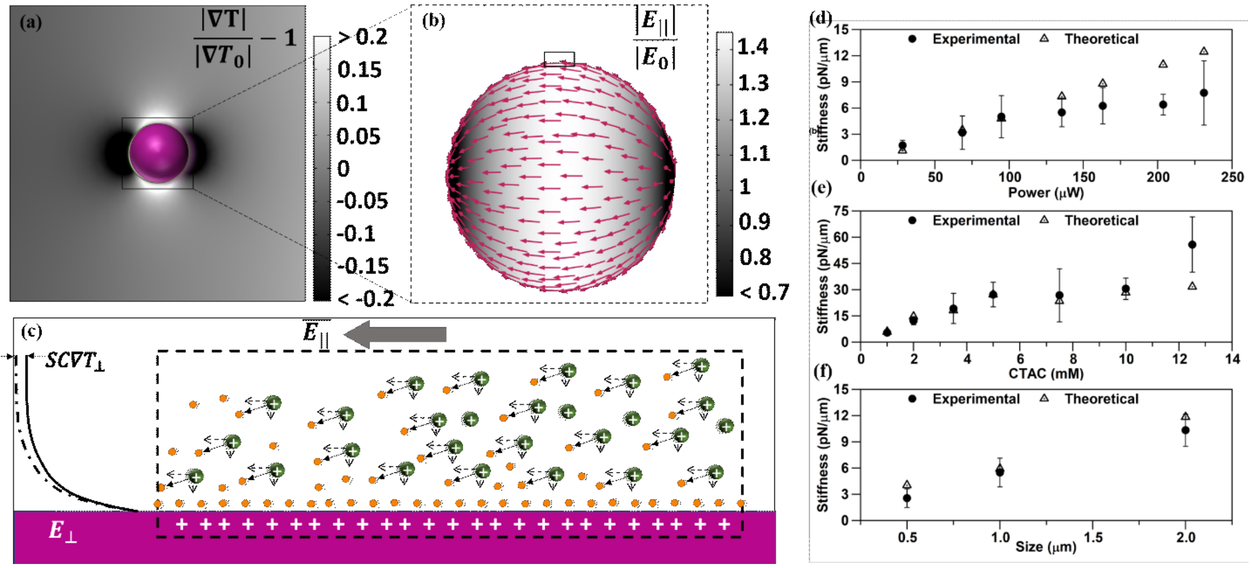

Figure 1 Theory of thermoelectric trapping and experimental validation: (a) Temperature gradient around the particle for a constant external temperature gradient. **(b)** Tangential component of the spatially varying thermoelectric field on the particle. **(c)** Schematic of ion distribution around the particle surface indicating the Stern layer and dipole alignment causing the tangential component of thermoelectric field. **(d-f)** Experimental and theoretical trapping stiffness of PS particles as a function of laser power, CTAC concentration and particle size. (Default values of power, concentration and size are 135 μW, 1 mM and 1 μm respectively.

Since the current theoretical method includes the changing temperature gradient around the particle, the same can be extended to laser heating of particles. The theoretical predictions have been experimentally substantiated for diverse phenomena such as opto-thermoelectric trapping, rotation and pulling of particles. For opto-thermoelectric trapping, thermoelectric forces have been estimated and trapping stiffness of PS particles is determined for varying laser powers, surfactant concentration and size which match well with the experimental values (Fig. 1d-f). The phenomenon of opto-thermoelectric pulling, obtained through self-heating of Silica particles, is well-explained from the balance between thermoelectric and optical forces. Also, the in-plane rotation of Janus particles under laser illumination was understood through explicit evaluation of thermoelectric and Stokes resistance torque.

3. Conclusions:

From the proposed theory, assisted with flexible modelling of the theory, we believe that this model has distinct advantages over mathematical models in terms of applicability to diverse experimental phenomenon. Moreover, shape-variations can easily be included in this theory by building the particle in any commercial 3D modelling software. Although the focus in this work has been on laser-induced thermoelectric fields, this model will also be valid for generic thermoelectric fields. With such flexibility in involving material, shape, size and composition of particles, and 3D spatial variation of electric fields around the particles to study particles' interactions, our computational model bridges down the gap considerably between the existing theory and experimental observations, thereby suitable for optimization studies in nanorobotics, nanophotonics and cellular biology.

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