

Exploring the limit of multiplexed near-field optical trapping

Donato Conteduca¹, Giuseppe Brunetti², Giampaolo Pitruzzello¹, Francesco Tragni², Kishan Dholakia³, Thomas F. Krauss¹, Caterina Ciminelli^{*,2}

¹ Photonics Group, Department of Physics, University of York, Heslington, York YO10 5DD, UK

² Optoelectronics Laboratory, Politecnico di Bari, Via E. Orabona 6, 70125, Bari, Italy

³ SUPA, School of Physics & Astronomy, University of St Andrews, KY16 9SS, UK

* Corresponding Author: caterina.ciminelli@poliba.it

Supplement: Exploring the limit of multiplexed near-field optical trapping

S1. Design of the metasurface with a parametric analysis on the gap g and the hollow core b

We simulated the properties of the metasurface with a 3D Finite Element Method solver (COMSOL®). We carried out a parametric analysis on the gap g and the hollow core of the nanocuboid b to calculate the values of Q -factor and resonance amplitude. Both parameters contribute to the optical forces, yet a trade-off between them is typically observed. For example, increasing b and reducing g provides the highest Q -factor, but at the expense of resonance amplitude; as a case in point, a Q -factor of 2.5×10^3 is obtained with $b = 120$ nm and $g = 50$ nm, but with a reflectance amplitude of only $R = 0.05$. We therefore choose $b = 120$ nm and $g = 90$ nm, which achieves $Q \sim 10^3$ and $R = 1$ and represents the best compromise for the trapping efficiency, as we discuss in section 2.1. In addition, the size of the hollow core $b = 120$ nm is favourable for objects of ≈ 100 nm size such as viruses, which is the type of trapping object considered here. In general, a smaller value for g will increase the Q -factor but decrease the amplitude, while reducing b will make it more difficult to trap the desired size of object. For a different size of trapped objects, a different design of the metasurface should be considered to optimize the trapping efficiency overall.

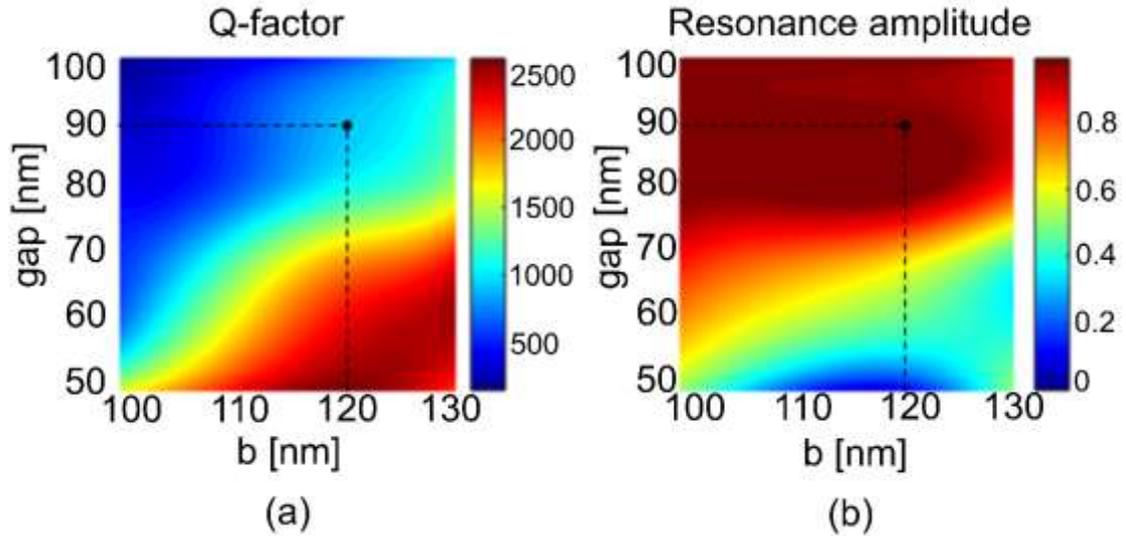


Figure S1. (a) Q -factor and (b) resonance amplitude as a function of the gap g and the hollow core b , assuming a period $A = 430$ nm and a thickness $t = 100$ nm for each nanocuboid.

S2. Comparison of resonance performance for different array size

We investigated the optical response of the array as a function of array size by fabricating different size arrays, ranging from 50x50 to 500x500. We note that the reflection spectrum of the large array ($N > 500$), that we consider infinite, provides very similar performance to an array of $N = 100$. Due to fabrication limitations, usually the shape of the nanostructures at the edge of the array is not homogeneous, which in practice confirms that the array size that is contributing to the resonance is $N < 100$, in good agreement with the numerical results shown in Fig. 3 in the main manuscript.

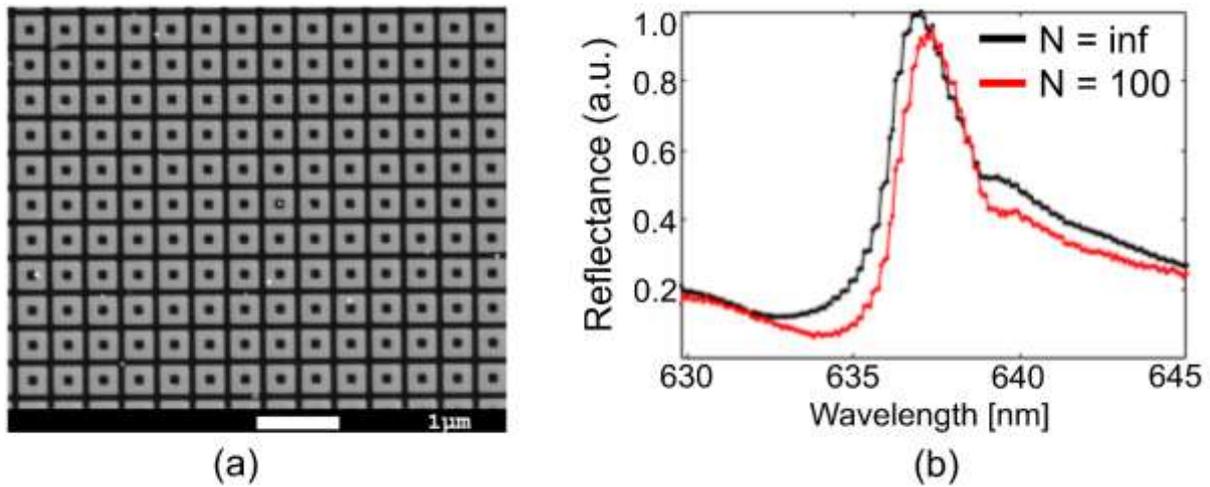


Figure S2. SEM micrograph of a section of a large array of nanocuboids, assuming N very high ($N=\text{infinite}$) and (b) reflection spectra for $N = \text{inf}$. (black curve) and $N = 100$ (red curve).

S3. Impact of adjacent traps on a single site for dynamic multiple trapping

We have also studied the impact of one particular optical trap on the adjacent trapping sites, in order to understand how the surrounding environment affects the trapping strength in each trapping site.

The simulation assumes the parameters of the nanocuboid structures as fabricated (Figure 4), assuming $b = 115$ nm, $g = 95$ nm and rounded corners with a curvature radius of 15 nm (Figure S3b). In figure S3a, we show the resonance spectrum of the array for the case when all traps are empty (black curve) and when all traps are filled (red curve), observing a resonance shift of $\Delta\lambda = 1.05$ nm and a change in reflectance of $\Delta R = 0.55$. Then, we have calculated the resonance response with only partially filled traps, observing a linear behaviour of the resonance shift by increasing the number of traps occupied, which is due to the increase of the effective index in each single filled trap (Figure S3c).

This study helps to understand the impact of adjacent traps on a specific trapping site. The operating wavelength is chosen to match the resonance condition of the metasurface when all trapping sites are occupied, which achieves maximum trapping strength due to the self-induced back-action (SIBA) effect (Figure S3d). For a high concentration of biological targets, this choice is reasonable because the probability that a large number of trapping sites can be easily filled simultaneously is high. This observation confirms that when an empty trapping site is filled, the adjacent sites benefit because of the favourable resonance shift experienced by the ensemble.

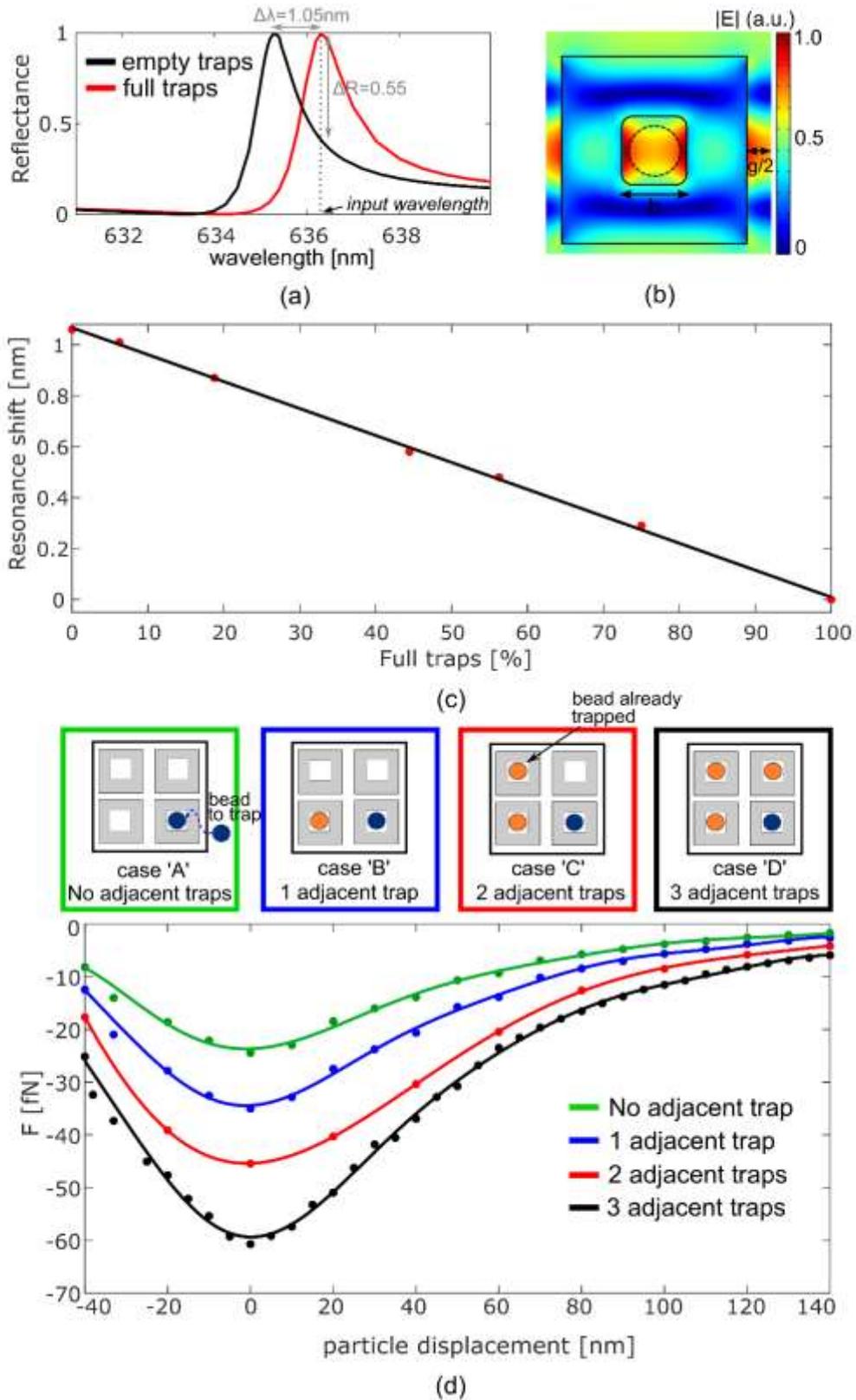


Figure S3. (a) Reflection spectra of the metasurface, considering the fabrication tolerances ($b = 115 \text{ nm}$, $g = 95 \text{ nm}$ and curvature radius of 15 nm of the nanocuboid core) when all traps are empty (black curve) and when all traps are full (red curve). (b) Mode distribution on resonance when the trap is occupied by a 100 nm bead of refractive index $n = 1.45$. (c) Resonance shift vs. number of filled traps of the metasurface array. (d) Optical forces obtained with $P = 7 \mu\text{W}/\text{cell}$ on a single particle being trapped in a unit cell of the metasurface (blue circle in the schematic) for a different number of particles already trapped in the adjacent unit cells (orange circles).

S4. Optical forces for different particles size

Finally, we calculated the optical forces exerted on particles in a range of sizes, around 100 nm, to account for natural size fluctuations. For example, the most common viruses (e.g. influenza virus and coronavirus) present a typical size of $100 \text{ nm} \pm 20 \text{ nm}$ ^{32,33}. We therefore study particles with a diameter of 80 nm, 100 nm and 120 nm. As expected, the optical forces scale with particle volume.

The designed metasurface confirms the ability to trap also particles with $D = 120 \text{ nm}$, however for larger particles a different design with a larger core should be considered.

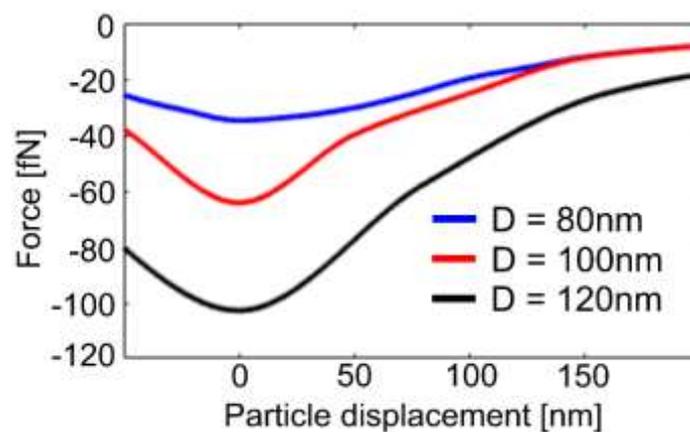


Figure S4. Optical forces exerted on particles with a diameter of 80 nm (blue curve), 100nm (red curve) and 120nm (black curve).