

Structures resistant to manipulation by all wavefronts in two dimensions

Asher Sabbagh¹, Michael Horodyski^{1,2,*}, Rida Khan¹, Brian Shi¹, and Marin Soljačić^{1,3}¹Department of Physics, *Massachusetts Institute of Technology*, Cambridge, Massachusetts 02139, USA²Photonics Institute, *Vienna University of Technology (TU Wien)*, Vienna A-1040, Austria³Research Laboratory of Electronics, *Massachusetts Institute of Technology*, Cambridge, Massachusetts 02139, USA

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Using light to manipulate small particles is a powerful tool with numerous practical applications across biophysics and nanotechnology. This experimental technique has achieved significant performance gains by employing shaped wavefronts, most commonly generated with spatial light modulators. Wavefront shaping has also enabled the manipulation of seemingly arbitrary objects beyond the reach of conventional beams. Contrary to this established assumption, we show here the existence of a wide variety of objects resistant to manipulation, even with the optimal wavefront shaping protocol. The counterintuitive shapes of these objects are found using inverse design in two dimensions, providing a foundation for their natural extension to three dimensions. Specifically, we show that the maximal pulling force is reduced by up to 4 orders of magnitude, and the maximal trapping stiffness is reduced by up to nearly 2 orders of magnitude. Our findings could prove useful for the development of micromachines that require a predictable mechanical response to arbitrary waves.

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I. INTRODUCTION

Since the pioneering work of Ashkin, who first demonstrated that tightly focused light can stably trap microscopic particles [1], optical micromanipulation has developed into a versatile tool across physics, biology, and soft matter [2–4]. For example, optical trapping has been used to elucidate the biomechanics of biological processes [5,6], control micromachines [7,8], experimentally validate the connection between entropy and information [9,10], and aid in cooling nanoparticles to their motional ground state [11,12]. The same optical fields can also transfer angular momentum [13] and even generate pulling forces [14,15]. Related capabilities also exist in acoustics, including acoustic tweezers for manipulating single microparticles, cells, and entire organisms [16] and acoustic tractor beams [17].

The ability to shape the wavefront of light [18–21] beyond the conventionally used Gaussian beams has advanced micromanipulation capabilities [22,23]. For example, wavefront shaping enables trapping behind scattering layers [24], stiffer traps [25,26], controlled transfer of angular momentum [27], trapping at multiple spots [28], and trapping and manipulating rod-shaped bacteria [29]. Alternatively, the near field around the particle can be tailored by inverse designing nanocavities and plasmonic apertures [30,31]. Acoustic transducer arrays provide an analogous form of control and can, for example, drive objects even through disordered and

dynamic media [32]. A complementary route for improving micromanipulation performance is inverse designing particles for fixed wavefront illumination (commonly a plane wave or Gaussian beam) [33–35]. Bounds on optimal forces, torques, and illumination fields [36,37] solidified the understanding that shaped waves have a large influence for manipulating objects. These successes raise a fundamental question: Are there targets for which mechanical control remains fundamentally limited even with optimal wavefront shaping?

In this paper, we identify targets for which even the optimal incident wavefront cannot efficiently realize certain micromanipulation tasks. We inverse design structures whose mechanical response is predictable for an arbitrary wavefront (within fixed illumination constraints). As one example, we numerically show that the maximum achievable pulling force (“optimal tractor beam”) on these inverse-designed targets can be suppressed by up to 4 orders of magnitude relative to a generic structure with a uniform refractive-index distribution. Remarkably, the ability to design such structures persists across broad parameter ranges, indicating that wavefront shaping does not guarantee arbitrary mechanical control. Our results not only show that it is possible to find structures that are predictably manipulated by an arbitrary wave, enabling reliable micromanipulation with dynamically distorted wavefronts. They also demonstrate that wavefront shaping does not guarantee arbitrary mechanical control, as we establish numerically over a broad parameter range.

II. INVERSE DESIGN OF MANIPULATION-RESISTANT STRUCTURES

To inverse design structures where the optimal wavefront exhibits a negligible influence on the target, we first need the ability to compute the optimal wavefront. For the first example of targets designed for greatly reduced optimal pulling forces,

*Contact author: michael.horodyski@tuwien.ac.at

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we employ the generalized Wigner-Smith (GWS) operator Q_x , which was introduced for optimal focusing on targets in disordered media [38] and has in the meantime been applied to a wide range of manipulation tasks [26,39–41]. The optimal tractor beam wavefront is found by solving the eigenvalue problem of Q_x (which is Hermitian in the absence of loss and gain in the system) for the largest eigenvalue, which reads

$$Q_x \bar{u}_x = (K_x^{\text{in}} - S^\dagger K_x^{\text{out}} S) \bar{u}_x = q_x \bar{u}_x, \quad (1)$$

where S is the target's scattering matrix, K_x^{in} (K_x^{out}) describes the incoming (outgoing) momentum of an arbitrary wavefront, $\bar{u}_x$ is a vector of modal amplitudes, and q_x is the eigenvalue. From this equation, we can interpret Q_x as describing the difference between the wave's incoming and outgoing momentum, which is transferred (by conservation of momentum) to the target. We restrict our analysis to two spatial dimensions, where the scattering of waves is governed by the Helmholtz equation $[\Delta + k^2 n^2(\mathbf{r})]\psi(\mathbf{r}) = 0$, with Δ the Laplacian, $k = |\mathbf{k}|$ the wave vector, $\psi(\mathbf{r})$ the scalar wave, and $n(\mathbf{r})$ is the spatially varying refractive index (which is continually adjusted during the inverse design process). We solve the two-dimensional Helmholtz equation numerically using our publicly available code [42] based on an open-source finite-element method (NGSolve) [43,44]. We note that the pipeline from scattering matrix to optimal wavestates can be extended to three dimensions if separate modal amplitudes for each polarization are included, and the scattering matrix takes polarization mixing into account. However, going to three dimensions incurs substantially increased computational cost, necessitating nonstandard simulation approaches [35,45].

Our ultimate goal is to find structures for which the largest eigenvalue of Q_x , q_x^{max} is vanishingly small [see Fig. 1(a)]. Since this eigenvalue gives—for all possible incoming wavefronts—the largest pulling force (i.e., the strongest tractor beam), $q_x^{\text{max}} \sim 0$ implies that it is impossible to pull the target with *any* wave. We achieve this goal by employing inverse design [see Fig. 1(b)], in which we continuously adjust the refractive-index distribution of the structure (parametrized by a square grid of pixels with individually tunable refractive indices between a minimum and maximum value) guided by a cost function (which is just q_x^{max}). To use state-of-the-art gradient-based inverse design algorithms, we require a computationally efficient way of calculating the gradient of the cost function with respect to the refractive index, n_i , of each design pixel, i.e., $\partial_{n_i} q_x^{\text{max}} = (\bar{u}_x^{\text{max}})^\dagger \partial_{n_i} Q_x \bar{u}_x^{\text{max}}$. From Eq. (1), we see that calculating $\partial_{n_i} Q_x$ amounts to the computation of $\partial_{n_i} S$, since K_x is independent of the refractive-index distribution. We efficiently calculate the sensitivity of the scattering matrix with respect to the refractive indices of the design pixels by using a method based on an alternative form of the generalized Wigner-Smith operator naturally suited to the task at hand [46]. We refer to the Appendixes for a detailed description of the gradient computation and inverse design algorithm.

In Fig. 1, we show the resulting structure of one such design run and compare its performance to that of a conventional structure. More specifically, we place a square design region ($\sim 1.8\lambda \times 1.8\lambda$) with a grid of 183×183 design pixels

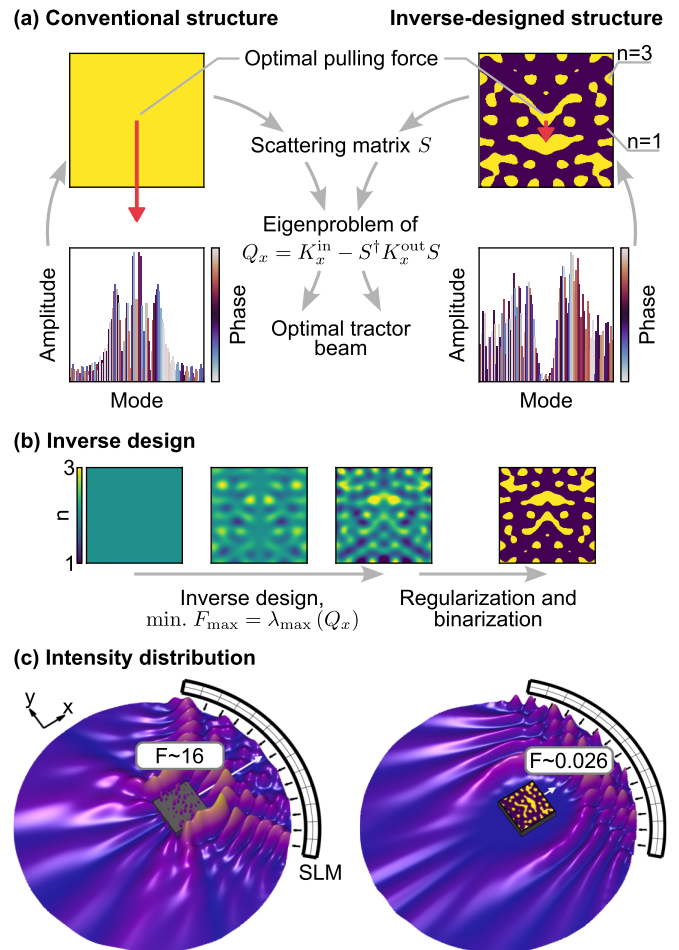


FIG. 1. Reduction of optimal tractor beam strength with inverse design. (a) Refractive-index distribution of a conventional structure (left) with a uniform refractive-index distribution ($n = 3$) and an inverse-designed structure that minimizes the optimal pulling force (right). In both cases, the wavefront exerting the optimal tractor beam (shown in amplitude and phase by the colored bar plots) is the extremal eigenvector of the generalized Wigner-Smith operator Q_x . (b) Sketch of the inverse-design procedure that iteratively changes the refractive-index distribution in a design region to minimize the optimal pulling force, i.e., the largest eigenvalue λ_{max} of Q_x . Here, we binarize the structure and smooth its boundaries, upon settling in a local minimum. (c) Comparing the intensity distribution of an optimal tractor beam for a conventional structure (left) and an inverse-designed structure (right). Our inverse-design procedure results in an optimal pulling force F reduced by nearly 3 orders of magnitude compared to the conventional structure. We restrict the aperture of the incoming wave to one-quarter of the circular boundary. The gray square indicates the extent of the design region.

in the middle of a circular scattering region. We can inject wavefronts into the scattering region with an arbitrary amplitude and phase distribution in a $\pi/2$ solid angle. These wavefronts always have unit norm for comparable results, i.e., $\bar{u}^\dagger \bar{u} = 1$. Our simulations reveal an optimal pulling force on the conventional structure (a square with a uniform refractive index of $n = 3$) of $F_x \sim 16$ (a.u.). In contrast, the optimal pulling force on the inverse-designed structure is smaller by nearly 3 orders of magnitude: $F_x \sim 0.026$ (a.u.). We note that

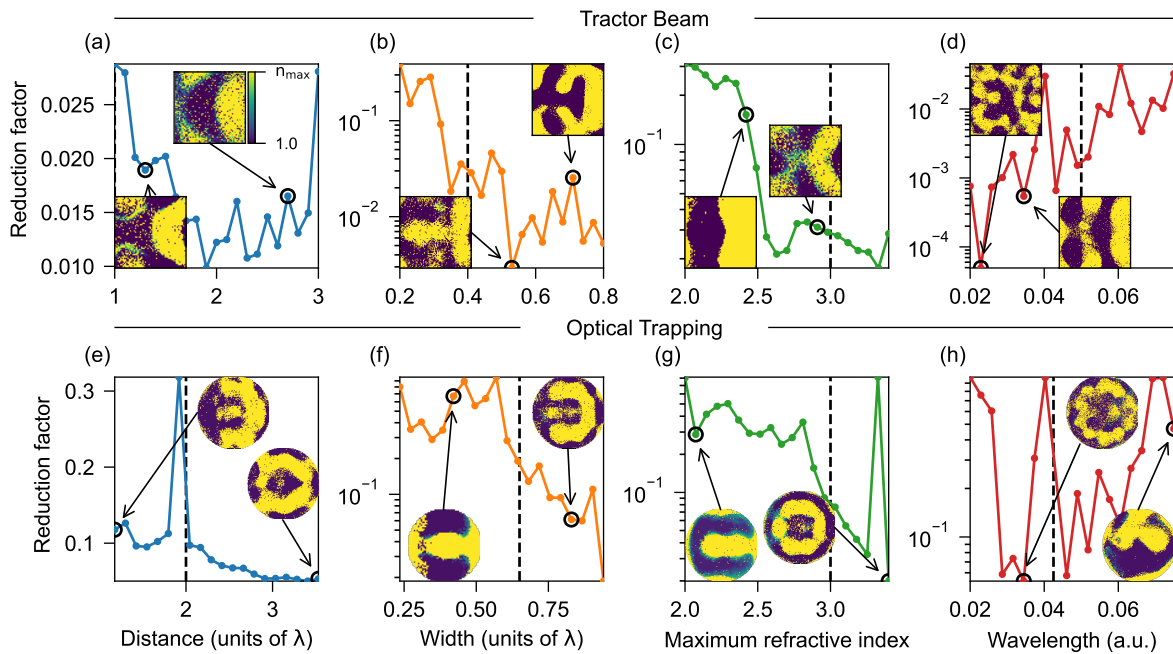


FIG. 2. Broad parameter range for tractor beam- and trapping-resistant particles. Plots show by how much the optimal micromanipulation has been reduced for an inverse-designed target compared to a conventional structure with a uniform refractive index. The top row and bottom give the reduction factor for the optimal tractor beam (i.e., the largest eigenvalue of Q_x) and optimal trapping stiffness (i.e., the largest eigenvalue of W_x), respectively. The reduction factor is shown as a function of distance [panels (a) and (e)], design-region width [panels (b) and (f)], maximal refractive index of the structure [panels (c) and (g)], and wavelength [panels (d) and (h)]. Insets show examples of inverse-designed structures that minimize this ratio. The black dashed line indicates the parameter value used in the other scans. The only exception is the wavelength scans, which are performed at a width of 0.04 a.u. to also investigate structures larger than a single wavelength.

the wave's ability to apply a pushing force is (in principle) unaffected by our design procedure. In this example, the maximal pushing force on the inverse-designed [conventional] target is $F \sim -653.1$ (a.u.) [$F \sim -457.6$ (a.u.)].

III. TRACTOR BEAM-RESISTANT STRUCTURES

Having presented one example of an inverse-designed structure where the optimal pulling force is reduced by 2 orders of magnitude, we now turn our attention to the question of whether such structures can be found generically. To this end, we vary the parameters of the studied system and investigate the extent to which the optimal pulling force is reduced relative to that of a corresponding conventional structure. Concretely, we sweep the distance of the structure to the wave's source, the side length of the square design region, the maximum refractive index, and the wavelength. We note that each structure is designed for one particular wavelength, i.e., for monochromatic illumination, and that changing the distance of the structure to the source also indicates the influence of varying the numerical aperture.

Our results are summarized in Figs. 2(a)–2(d) and clearly show that structures (strongly) resistant to the optimal pulling force occur over a wide range of parameters. This indicates that we have identified a large class of structures and that wavefront shaping does not, in general, guarantee arbitrary micromanipulation capabilities. Our data also clearly indicate that reducing the effective size of the design region (either by

changing the size itself or indirectly by increasing the wavelength or decreasing the maximal refractive index) reduces the inverse-design algorithm's ability to identify structures that perform markedly better than conventional structures. Intuitively, this observation is explained by the transition to purely dipole scattering for targets that are much smaller than the wavelength. In this case, the patterning is not resolved by the wave; thus, inverse design loses its influence on the optimal pulling force. These observations remain consistent if we restart the inverse design process with a different set of randomly selected refractive indices within the design region, indicating robustness to initialization. The wavelength scan is performed at a width of 0.04 a.u. to also include design regions up to $2\lambda \times 2\lambda$ in size. Even at these sizes, we can design structures resistant to manipulation by up to 4 orders of magnitude compared to a conventional structure. This is especially remarkable since, for large structures, wavefront shaping usually exhibits improved performance compared to smaller structures [25,26].

In the Appendixes, we study the robustness of a representative sample of the inverse-designed structures to fabrication uncertainties. Our simulations reveal that the observed effect of manipulation resistance breaks down for root mean square fabrication errors >0.2 . This particular value approximately corresponds to changes in the structures that are on the order of $\lambda/10$. Furthermore, we show in the Appendixes that manipulation resistance breaks down completely for a change in wavelength larger than $\lambda/10$. This indicates that our results

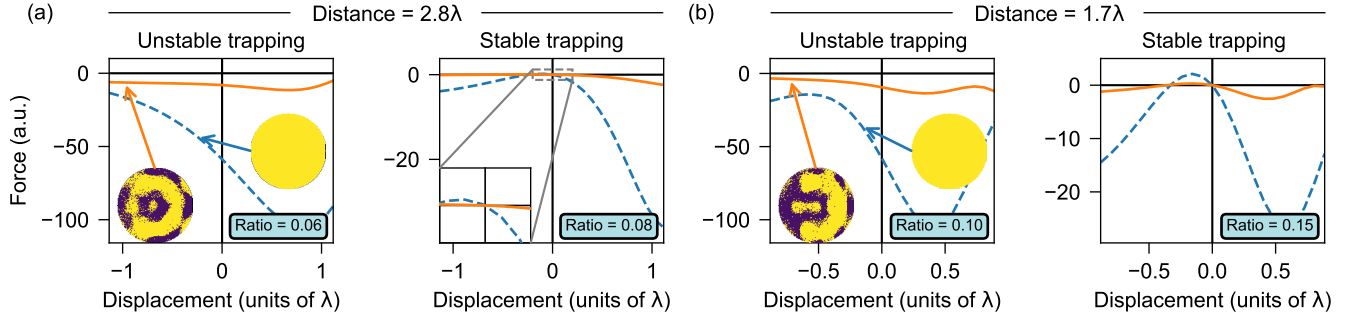


FIG. 3. Maximum trapping stiffness and stable trapping. Force exerted as a function of displacement from the initial position for two different initial positions [(a) 2.8λ and (b) 1.7λ , respectively]. In both cases, we compare the response of both the inverse-designed structure (for small optimal trapping stiffness) and the conventional structure with a uniform refractive-index distribution. Furthermore, we apply two different wavefronts [left and right sides in panels (a) and (b), respectively]. One produces the optimal trapping stiffness as it corresponds to the largest eigenvalue of W_x , while the other maximizes the trapping stiffness under the constraint of stable trapping. Insets show the structures used and the ratio of the trapping stiffness between the inverse-designed and conventional structures by computing the ratio of the slopes at 0 displacement.

rely on interferometric effects, since they are usually sensitive to this scale.

IV. STRUCTURES RESISTANT TO OPTICAL TRAPPING

We now show that the inverse design of structures resistant to manipulation also extends to the optical trapping of particles. Accordingly, we use an operator derived from the generalized Wigner-Smith operator in Eq. (1) that allows us to compute the wavefront with the optimal trapping stiffness. The trapping stiffness (in x direction) $\kappa_x = -\partial_x F_x$ quantifies how tightly a particle is trapped by computing how quickly a restoring force builds when the particle is displaced from its equilibrium position. The corresponding operator is given by [26]

$$W_x = -\partial_x Q_x = i(S^\dagger K_x^{\text{out}} S K_x^{\text{in}} - K_x^{\text{in}} S^\dagger K_x^{\text{out}} S), \quad (2)$$

where we used $\partial_x S = i(S K_x^{\text{in}} - K_x^{\text{out}} S)$ [38] to arrive at W_x . Since the only part of W_x that depends on the refractive index of the design pixels is the scattering matrix S , we employ the same inverse design strategy as for the tractor beam case. Here, we use a circular design region to connect our results to optical trapping experiments, which usually employ silica nanospheres as targets. This also means that the conventional structure used as the baseline is circular and has a uniform refractive-index distribution.

For structures designed to resist an optical trapping beam, we find a wide range of parameters in which the performance of the optimal trapping beam degrades by up to 2 orders of magnitude relative to a conventional structure [see Figs. 2(e)–2(h)]. The broad trend of larger structures performing better at resisting a trapping beam is similar to that observed for structures designed to withstand the optimal pulling force. Interestingly, with increasing distance to the wave's source, the performance of trapping-resistant targets improves, while the performance of tractor beam-resistant targets stays unchanged. In both micromanipulation examples considered here, the structures identified by our inverse-design process consist primarily of two materials, as we employed hyperbolic-tangent regularization to guide the opti-

mizer toward solutions exhibiting this property. The structures also exhibit comparably smooth boundaries without nudging them toward this property in the inverse-design process.

However, in optical trapping, it is usually not sufficient to only target improved trapping stiffness with wavefront shaping [4]. Rather, great care has to be taken to ensure that a trap is not only stiff, but also stable; i.e., no force is applied at zero displacement ($x = 0$). In our case, this means that the trapping beam should not only maximize $\vec{u}^\dagger W_x \vec{u}$, but also ensure that $\vec{u}^\dagger Q_x \vec{u} = 0$ at the equilibrium position, where $\vec{u}$ is the optimal wavefront. We find wavestates that possess these two properties by numerical optimization (see Appendixes for a detailed description of the procedure), as no simple eigenproblem is available to compute the corresponding wavefront [26].

We analyze the response of conventional and inverse-designed structures to wavefronts that maximize trapping stiffness while keeping the trap stable in Fig. 3. Our results reveal that changing the wavefront from one that just maximizes trapping stiffness to one that also results in stable trapping does not adversely affect the purpose of the inverse-designed structure; i.e., the optimal trapping stiffness is still reduced by approximately an order of magnitude, and the potential well created by the optical trap is much shallower for the inverse-designed structure.

V. DISCUSSION AND OUTLOOK

A remaining question is whether the reduction factors R reported here would have a practical effect in an experiment. To this end, we consider a standard optical tweezer experiment (a micrometer-sized silica sphere immersed in water resulting in Brownian motion) with the addition of a spatial light modulator that enables wavefront shaping to optimize manipulation figures of merit [26]. For this experiment, we use the publicly available code of Ref. [26] to compute key quantities such as optimal tractor beam strength and trapping potential depth for a beam with optimal trapping stiffness.

For a tractor beam, we determine the timescale required to distinguish the effect of a pulling force from Brownian motion by considering the time required to observe a change in the

average position of the target larger than one standard deviation: $t^* = 2\gamma k_B T / (\mathcal{R}_F R P)^2$ (we provide a detailed argument in the Appendixes). Here, R is the reduction factor, $\mathcal{R}_F \approx 0.71 \text{ nN/W}$ the optimal tractor force per Watt laser power, P the laser power, γ the particle friction, k_B the Boltzmann constant, and $T = 300 \text{ K}$. For example, for $R = 5.9 \times 10^{-4}$ and $P = 1 \text{ mW}$, the time is $t^* = 1 \text{ h}$.

In the case of an optical trap, the behavior of trapped particles can be estimated by comparing the depth of the potential well, $\Delta U = \mathcal{R}_{\Delta U} R P$ ($\mathcal{R}_{\Delta U} = 0.098 \text{ fJ/W}$ is the potential depth per Watt laser power), to the thermal energy $k_B T$. If $\Delta U > 10k_B T$, then the particle stays trapped indefinitely. For $\Delta U > k_B T$, the particle is confined for a short time (on the order of minutes) and then ejected from the trap, while for $\Delta U < k_B T$ it is only weakly influenced by the optical tweezer and primarily experiences free diffusion. To confirm these estimates, we simulate the motion of a particle in the force field of an optimally stiff trap [in one dimensional (1D)] subject to a stochastic force (i.e., Brownian motion). We use these simulations to compute the time it takes for the particle to be ejected from the trap and confirm the approximations above (see the Appendixes).

To summarize, we have inverse-designed structures that are resistant to pulling forces and optical trapping beams, even when the *optimal* wavefront for the task at hand is used. We illustrated the viability of our concept with numerical simulations, reducing the capability to manipulate inverse-designed structures by up to 4 orders of magnitude relative to conventional structures. The properties of targets we found potentially enable the application of our inverse-design pipeline to the fabrication of structures suited both for optical [35] and acoustic [34] micromanipulation. Although the results presented here are for a two-dimensional (2D) system, the extension to three-dimensional (3D) vector waves should be possible. Since our findings uncover that increasing the number of modes facilitates designing manipulation-resistant targets, we do not expect that the increased mode space in 3D will be a hindrance.

Our approach offers an interesting perspective on optically driven micromachines [47], when only specific degrees of freedom need to be addressed. It potentially enables the operation of such micromachines even when they are embedded in a disordered, changing environment, i.e., when the illuminating wavefront is constantly evolving. Manipulation-resistant structures could also be used to reduce backaction noise in optical levers [48].

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DATA AVAILABILITY

The code used for this study is freely available in Ref. [42].

APPENDIX A: EXTRAPOLATING TO THREE DIMENSIONS

Here, we reinterpret the data in Fig. 2 and investigate how the reduction factors scale with the number of scattering channels and the resolved feature size. In this way, we argue that an increase of the number of scattering channels when going from 2D to 3D, as well as the increase in resolved feature size, is not expected to be a major hindrance.

The data in Fig. 4 show that, in most cases, an increase in the number of scattering channels, as well as larger resolved features, decreases the reduction factor. The only exception is in the optical trapping case, where an increase in the number of scattering channels does not meaningfully affect the reduction factor. Since the modal amplitudes for the incoming wavefront are proportional to $1/H_n^{(1)}(kR)$, which for $n > kR$ is approximately zero, the number of scattering channels is given by $\sim kR$.

APPENDIX B: MANIPULATION-RESISTANT STRUCTURES UNDER BROWNIAN MOTION

Here, we show the reduction factors required to render an inverse-designed structure manipulation resistant in a practical sense. To this end, we consider particles immersed in water that experience Brownian motion and investigate how weak manipulation can get before the Brownian motion becomes the dominant influence.

Tractor beam. The average position, μ , of a particle experiencing a constant pulling force, F , and Brownian motion time evolves as $\mu(t) = \frac{F}{\gamma}t$, where γ is the particle friction coefficient. The standard deviation, σ , of the position also evolves with time as $\sigma(t) = \sqrt{2Dt}$, with the diffusion constant given by $D = k_B T / \gamma$. To see whether the pulling force on a particle can be differentiated from Brownian motion on a feasible timescale, we define t^* as the time it takes for the average position to have moved 1σ :

$$t^* = \frac{2\gamma k_B T}{F^2}. \quad (\text{B1})$$

To investigate which reduction factors R result in impractically long t^* , we consider a representative system: a micron-scale dielectric bead (radius $a_{\text{bead}} = 4.01 \mu\text{m}$) suspended in water ($\eta = 10^{-3} \text{ Ns/m}^2$, $T = 300 \text{ K}$), for which the drag coefficient is $\gamma = 6\pi\eta a_{\text{bead}} \approx 7.6 \times 10^{-8} \text{ kg/s}$ and the diffusion constant of the Brownian motion is $D = k_B T / \gamma$ [49]. Using the publicly available code from Ref. [26], we estimate the optimal tractor force responsivity as $\mathcal{R}_F = F/P_{\text{laser}} \approx 0.71 \text{ nN/W}$. Then, t^* reads

$$t^* = \frac{2\gamma k_B T}{(R\mathcal{R}_F P_{\text{laser}})^2}. \quad (\text{B2})$$

We show in Fig. 5(a) the resulting t^* and observe that a $t^* = 1 \text{ h}$ is achieved with reduction factors, 5.9×10^{-3} , 5.9×10^{-4} , and 5.9×10^{-5} for laser powers 0.1, 1, and 10 mW, respectively.

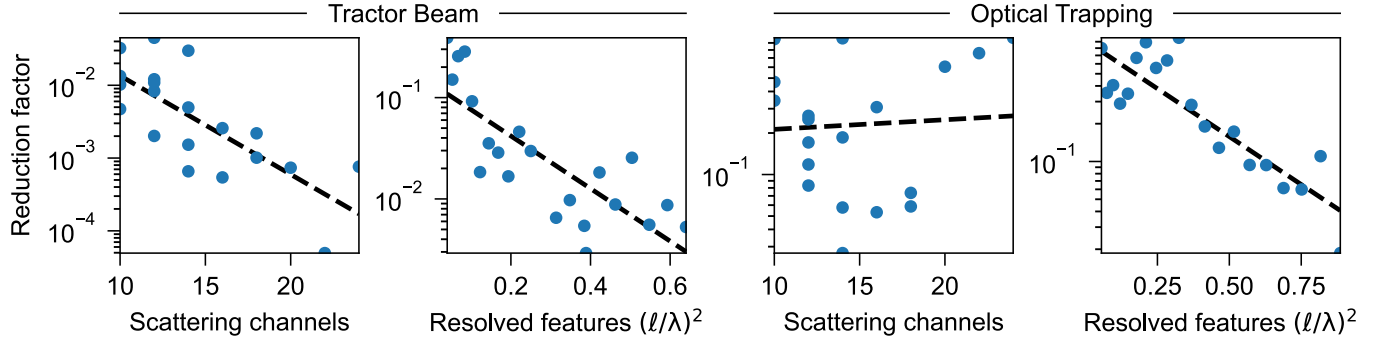


FIG. 4. Scaling of reduction ratios as a function of the number of scattering channels and resolved features for structures resistant to tractor beams and optical trapping, respectively. The number of scattering channels is $\sim kR$ in 2D and $\sim (kR)^2$ in 3D, respectively. The resolved feature size grows as $\sim (\ell/\lambda)^2$ in 2D and $\sim (\ell/\lambda)^3$ in 3D.

Optical trapping. To uncover which combinations of reduction factor and power result in particles being ejected from an optical trap due to Brownian motion, we use a simulated force over displacement curve [see Fig. 5(b)] [26]. Using this force field, we simulate the motion of a particle in 1D subject to a random force in the overdamped regime:

$$\frac{d}{dt}x(t) = \frac{1}{\gamma}F(x) + \sqrt{2D}W(t), \quad (\text{B3})$$

where $W(t)$ is white noise. If $|x| > 2a_{\text{bead}}$, we classify this as the particle being ejected from the trap and count the elapsed time as the trapping time.

We show in Fig. 5(c) the average trapping time of 200 runs as a function of laser power and reduction factor. The results fall into three different regimes: (1) The optical trap is too weak to meaningfully affect the particle, and thus the trapping time is mostly a result of how long the free diffusion process takes to reach the boundary ($\pm 2a_{\text{bead}}$). (2) The optical trap is strong enough to contain the particle for some time, but ultimately the particle is ejected from the trap. (3) The particle is trapped for more than 1 h (the time considered in the simulations). The border between regimes (1) and (2) is approximately given by $\Delta U(R, P) = k_B T$, where ΔU is the depth of the potential well, while the border between regimes (2) and (3) is approximately given by $\Delta U(R, P) = 10k_B T$.

APPENDIX C: SENSITIVITY TO WAVELENGTH VARIATIONS

Here, we investigate how inverse-designed structures respond to deviations from the design wavelength. Our primary insight is that inverse-designed structures show no difference from conventional structures (i.e., a reduction factor of ~ 1) in either their tractor beam strength or trapping stiffness after a $\sim 10\%$ change from the design wavelength (see Fig. 6). This suggests that the inverse-designed structures presented in this paper rely on interferometric effects, as these are also commonly associated with a $\sim 10\%$ sensitivity to parameter variations.

We arrive at this conclusion by considering all structures designed for both small tractor forces and low trapping stiffnesses in the case of a varying design wavelength [Figs. 2(d) and 2(h)]. For all these structures, we then simulated how the reduction factor changed as we varied the wavelength of the illuminating radiation.

APPENDIX D: FABRICATION UNCERTAINTY

We now discuss how sensitive the structures we generated are to inaccuracies in the fabrication process. We do this by considering two commonly encountered effects: We perturb

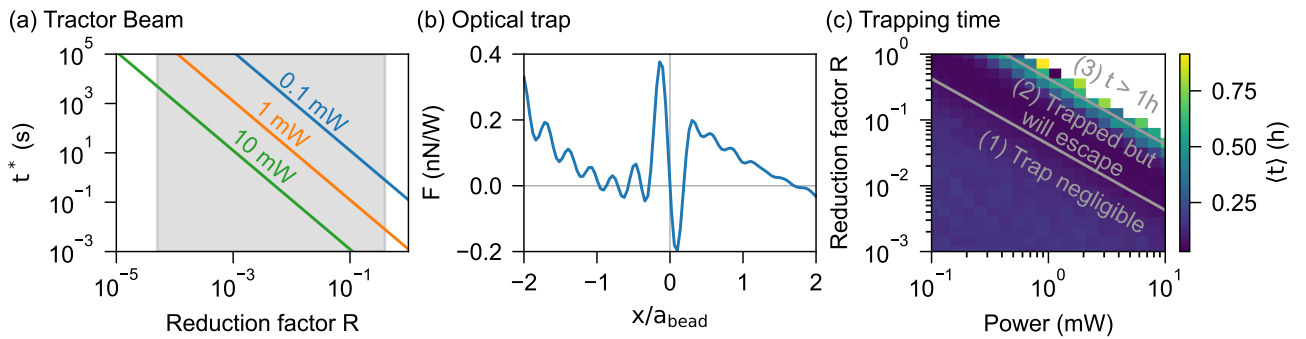


FIG. 5. Effects of Brownian motion. (a) Time to move average position by 1σ , t^* , as a function of reduction factor for various laser powers. The gray-shaded region marks the range of reduction factors found in Figs. 2(a)–2(d). (b) Force as a function of displacement for an optical trap in the longitudinal direction. The trapping stiffness of this trap is $\kappa = 10^3$ fN/nm for a 1 Watt laser. (c) Average trapping time, $\langle t \rangle$, as a function of laser power and reduction factor. Three distinct regimes emerge: (1) A trapping force weak enough to have negligible influence on particle movement, (2) a particle that is trapped but will escape after some time, and (3) a trapping time larger than 1 h (white region). The boundaries of the three regimes are $\Delta U(R, P) = k_B T$ and $\Delta U(R, P) = 10k_B T$, respectively.

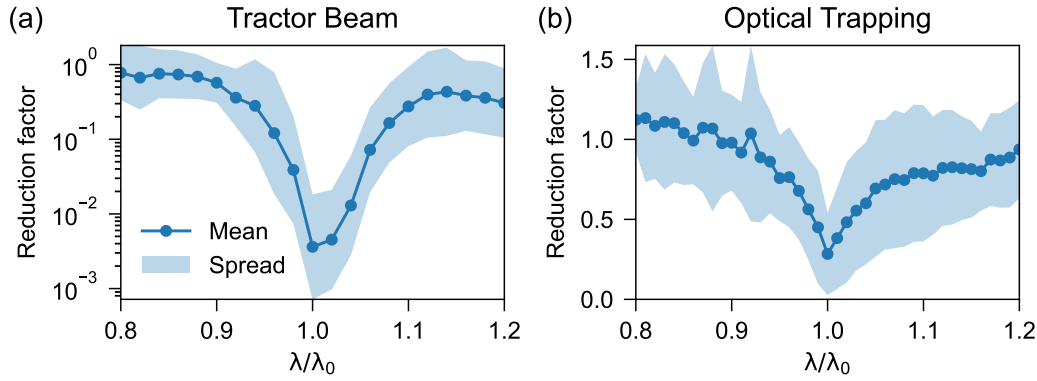


FIG. 6. Sensitivity of the reduction factor to wavelength changes. Reduction factor as a function of wavelength changes in the input field for both optimal tractor beams [panel (a)] and beams with optimal trapping stiffness [panel (b)]. To capture the main effects of this analysis across the 21 structures considered in both cases, we compute the mean and the one-standard-deviation spread. In the tractor beam case, we used both the logarithmic mean and standard deviation.

both the maximum refractive index and the edge roughness locally using a correlated standard normal distribution (see Fig. 7). We show the resulting changes in the reduction factor for selected structures from Fig. 2 in Figs. 8 and 9. To quantify the severity of the whole fabrication deviations, we use $\sigma_{\text{fab}} = \text{RMS}[n_{\text{fab}} - n_{\text{design}}]/(n_{\text{max}} - n_{\text{min}})$, where n_{design} is the original inverse-designed structure, n_{fab} is the structured including the fabrication errors, and n_{max} and n_{min} are the largest and smallest refractive index, respectively. The root-mean-square (RMS) is taken with respect to the spatial distribution of the error.

The main observation of Figs. 8 and 9 is that fabrication uncertainties start to have a noticeable effect on the reduction factor for $\sigma_{\text{fab}} > 0.2$. A notable exception can be seen in the case of structures that did not exhibit a small reduction factor, even for perfect fabrication: There, the change in the reduction factor is less noticeable with increasing fabrication errors, σ_{fab} . This allows us to conclude that the smaller the reduction factor, the more sensitive these structures are to errors in the fabrication process.

We also compare σ_{fab} to a length scale to get a better understanding of the scale of the fabrication uncertainties compared to the wavelength of the incoming laser. For small fabrication uncertainties, we can characterize σ_{fab} by the total change in area from the original structure to the fabricated one weighted

by refractive index:

$$\Delta A = \int_{\text{structure}} dA \frac{|n_{\text{fab}}(\mathbf{r}) - n_{\text{design}}(\mathbf{r})|}{n_{\text{max}} - n_{\text{min}}}. \quad (\text{D1})$$

From this comparison, we see that the value of σ_{fab} where the reduction factor grows rapidly (~ 0.2 for most structures) approximately corresponds to $\lambda/10$, which agrees with the Rayleigh criterion for minimum optical resolution.

APPENDIX E: SCATTERING THEORY

Here, we recap the work of Ref. [40] on calculating the scattering matrix in two dimensions with open boundary conditions. Our starting point is the homogeneous Helmholtz equation:

$$[\Delta + k^2 n^2(\mathbf{r})]\psi(\mathbf{r}) = 0, \quad (\text{E1})$$

where Δ is the Laplacian, $k = |\mathbf{k}|$ is the wave vector, $n(\mathbf{r})$ is the refractive-index distribution, $\psi(\mathbf{r})$ is the scalar wave, and $\mathbf{r}$ is the position. Written in polar coordinates (r, φ) , the most general free space solution is spanned by Hankel functions of the first and second kind:

$$\begin{aligned} \psi(\mathbf{r}) = \sum_{n \in \mathbb{Z}} [\alpha_n H_n^{(2)}(kr) + \beta_n H_n^{(1)}(kr)] \\ \times (\gamma_n e^{in\varphi} + \delta_n e^{-in\varphi}), \end{aligned} \quad (\text{E2})$$

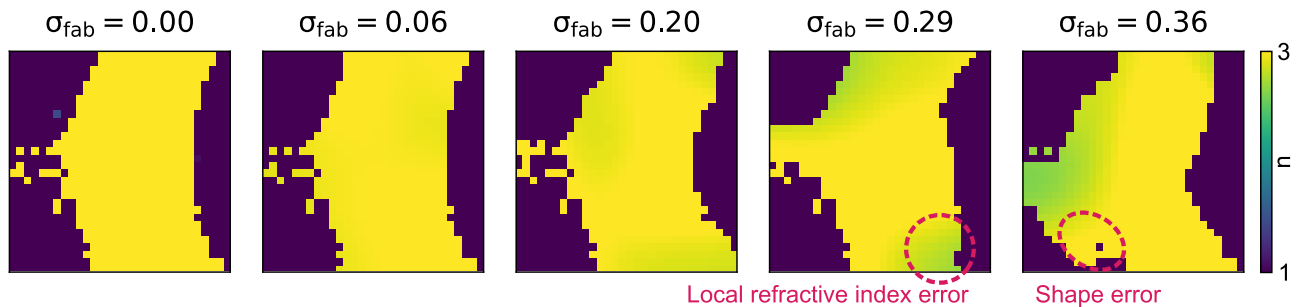


FIG. 7. Example of fabrication uncertainties. Refractive-index distribution of an inverse-designed structure with progressively severe fabrication errors quantified by σ_{fab} .

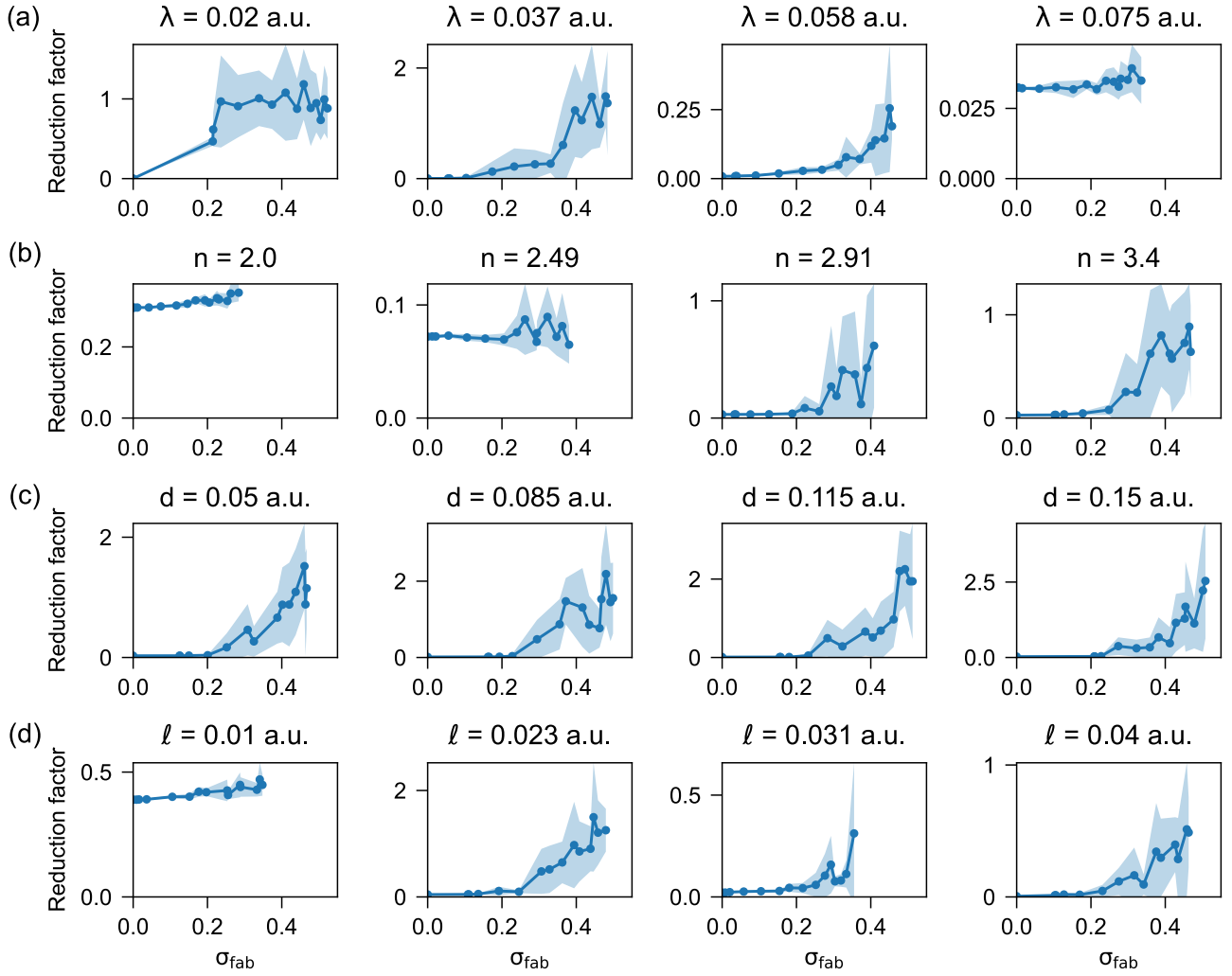


FIG. 8. Sensitivity to fabrication errors of structures resistant to pulling forces. Shown is the change in reduction factor of 16 representative devices as a function of the severity of fabrication error, σ_{fab} . We consider structures designed for different wavelengths λ [panel (a)], maximum refractive indices n [panel (b)], distances to the source of the waves d [panel (c)], and widths ℓ [panel (d)]. The solid line represents the mean over eight random realizations of fabrication errors, with the shaded region denoting one standard deviation.

where $\alpha_n, \beta_n, \gamma_n, \delta_n$ are the coefficients of the general expansion. This basis is complete and orthonormal, so we can use it to compute the matrix elements of a unitary scattering matrix, provided we restrict ourselves to flux-conserving systems (i.e., the absence of gain and loss). To arrive at a properly normalized expression for the scattering matrix, we consider the inhomogeneous Helmholtz equation with a source term $f(\mathbf{r})$:

$$[\Delta + k^2 n^2(\mathbf{r})]\psi(\mathbf{r}) = f(\mathbf{r}). \quad (\text{E3})$$

To excite an arbitrary incoming wave at the boundary of our design region $r = R$, we set $f(\mathbf{r}) = -\delta(r - R) \sum_n c_n e^{in\varphi}$, where c_n 's are the modal amplitudes. We then choose solutions inside and outside of the scattering region of the form

$$\psi_{\text{in}} = \sum_n a_n H_n^{(2)}(kr) e^{in\varphi}, \quad r < R, \quad (\text{E4})$$

$$\psi_{\text{out}} = \sum_n b_n H_n^{(1)}(kr) e^{in\varphi}, \quad r > R, \quad (\text{E5})$$

where a_n and b_n are expansion coefficients. We chose to study these forms of solutions because the norm of each component has a radial symmetry, which makes the source isotropic. We also note that all components have constant flux, so we can easily construct a flux-conserving scattering matrix from them by using these solutions to fix c_n 's from the source term [40]. To conserve the flux of our system, we enforce continuity of these solutions at $r = R$ to find that $a_n H_n^{(2)}(kR) = b_n H_n^{(1)}(kR)$. We can then plug these solutions back into Eq. (E3) to fix the source amplitudes, resulting in $c_n = -4ia_n/\pi R H_n^{(1)}(kR)$. Note that Hankel functions of constant argument but increasing n increase in their absolute value, so $|c_n|$ is decreasing with increasing n . This allows us to impose a heuristic cutoff to the number of modes, $n = N$, above which the modal amplitudes are effectively 0. Now that we know the full modal expansion of the source term, we can numerically compute the matrix elements of a unitary scattering matrix of an incoming cylin-

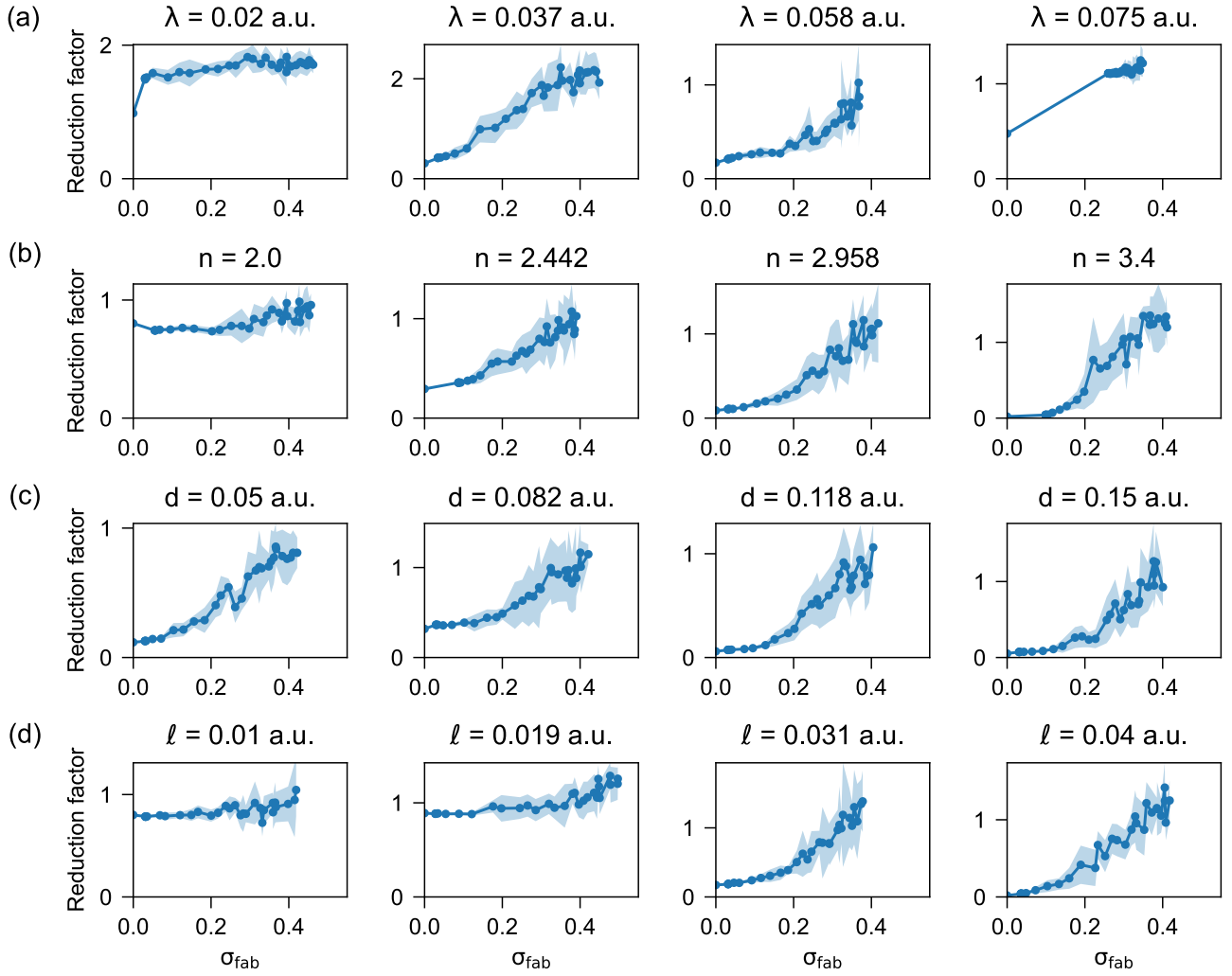


FIG. 9. Sensitivity to fabrication errors of structures resistant to optical trapping. Shown is the change in reduction factor of 16 representative devices as a function of the severity of fabrication error, σ_{fab} . We consider structures designed for different wavelengths λ [panel (a)], maximum refractive indices n [panel (b)], distances to the source of the waves d [panel (c)], and widths ℓ [panel (d)]. The solid line represents the mean over eight random realizations of fabrication errors, with the shaded region denoting one standard deviation.

drical wavefront with unit modal amplitude:

$$[S]_{mn} = \int_0^{2\pi} \frac{e^{in\varphi} \psi_n(R)}{2\pi H_m^{(1)}(kR)} d\varphi - \frac{H_n^{(2)}(kR)}{H_n^{(1)}(kR)} \delta_{m,-n}, \quad (\text{E6})$$

where the subtraction of the second term is to avoid double counting the incoming wave's contribution.

To compute the matrix elements of other relevant operators, we make use of the basis of incoming modes χ_n^{in} , by employing the fact that incoming waves are of the form $e^{in\varphi} H_n^{(2)}(kr)$ and normalizing. The basis wavefunctions are given by

$$\chi_n^{\text{in}} = \frac{e^{in\varphi} H_n^{(2)}(kr)}{\sqrt{2\pi |H_n^{(2)}(kR)|}}. \quad (\text{E7})$$

We can then write out the matrix elements of the incoming momentum operator in the x direction, K_x^{in} evaluated at the boundary:

$$[K_x^{\text{in}}]_{mn} = -i \int_0^{2\pi} d\varphi (\chi_m^{\text{in}})^* \frac{\partial}{\partial x} \chi_n^{\text{in}}, \quad (\text{E8})$$

where we note that $K_x^{\text{in}} = K_x^{\text{out}}$. By imposing our mode cutoff, the momentum operator is given by

$$[K_x^{\text{in}}]_{mn} = \frac{ik}{4} \left[\left(\frac{|H_n^{(1)}(kR)|}{|H_m^{(1)}(kR)|} + \frac{|H_m^{(1)}(kR)|}{|H_n^{(1)}(kR)|} \right) \delta_{m,n+1} - \left(\frac{|H_n^{(1)}(kR)|}{|H_m^{(1)}(kR)|} + \frac{|H_m^{(1)}(kR)|}{|H_n^{(1)}(kR)|} \right) \delta_{m+1,n} \right], \quad (\text{E9})$$

where m and n run from $-N$ to N . During our analysis, we restricted the incoming wavefront to an aperture of $\pi/2$. We achieve this by rewriting all relevant operators in the eigenbasis of the angular operator ϕ , and then simply setting components outside of the aperture to zero. Again, we use the basis of incoming modes to compute the matrix elements of ϕ :

$$[\phi]_{mn} = \int_0^{2\pi} (\chi_m^{\text{in}})^* \phi \chi_n^{\text{in}} d\varphi. \quad (\text{E10})$$

For Fig. 3, we need to compute the scattering matrix for a given structure at several positions. Rather than calculating the full scattering matrix from scratch at each of these points, which is computationally expensive, we compute the scattering matrix at a single position and then use the translation operator to evaluate it at any other position. This is the same translation operator used in standard quantum mechanics, generated by the momentum operator: $T(x) = e^{ixK_x^{\text{in}}}$, $T^\dagger(x) = e^{-ixK_x^{\text{out}}}$. To compute the scattering matrix at a distance Δx from the starting position, we use

$$S(x + \Delta x) = T^\dagger(\Delta x)S(x)T(\Delta x). \quad (\text{E11})$$

APPENDIX F: COST FUNCTION

1. Tractor beam micromanipulation

To proceed with our inverse-design procedure, we must define a cost function and compute its gradient to optimize the refractive-index distribution of our structure numerically. To generate structures that are resistant to a tractor beam, for example, we need a way to compute the force exerted onto the structure by the incoming wavefront and the gradient of that force under a change of the refractive-index distribution. To do this, we introduce the formalism of the generalized Wigner-Smith operators, because they allow us to calculate all relevant quantities in terms of operators evaluated at the boundary, like K_x^{in} and S . We define the GWS operator Q_α as [38,39]

$$Q_\alpha \equiv -iS^\dagger \frac{\partial}{\partial \alpha} S, \quad (\text{F1})$$

where α is some parameter of the system. We also define the scattering potential $U(\mathbf{r}) \equiv -k^2 n^2(\mathbf{r})$. Then, the GWS operator satisfies the following equation, which relates far-field information at the boundary to the optimization region [39]:

$$\vec{u}^\dagger Q_\alpha \vec{u} = \frac{-1}{2} \int dA |\psi_u(\mathbf{r})|^2 \frac{dU}{d\alpha}, \quad (\text{F2})$$

where $\vec{u}$ is the vector of modal amplitudes for some general incoming wavefront, $\psi_u(\mathbf{r})$ is the resulting solution to the Helmholtz equation inside the scattering region, and the integral is taken over the whole scattering region. To interpret Eq. (F2) in the case of $\alpha = x$, we use $\partial_x S = i(SK_x^{\text{in}} - K_x^{\text{out}}S)$ to arrive at a different form of the defining equation of Q_x :

$$Q_x \vec{u} = (K_x^{\text{in}} - S^\dagger K_x^{\text{out}} S) \vec{u} = q_x \vec{u}, \quad (\text{F3})$$

where q_x is the eigenvalue. Thus, we can interpret Q_x as describing the momentum difference between the incoming and outgoing waves. We note that this interpretation of Eq. (F3) is only true if it describes a single scatterer in an otherwise empty scattering region [38]. By choosing the eigenvector $\vec{u}_{\text{max}}$ whose associated eigenvalue q_x^{max} is largest, we can perform minimization on it to ensure that the force is minimal for an arbitrary incoming wavefront.

We compute the gradient of q_x by observing how an eigenvalue variation corresponds to a variation in the operator:

$$dq_x = \vec{u}^\dagger dQ_x \vec{u}. \quad (\text{F4})$$

To vary Q_x , we consider Eq. (F3) and arrive at

$$dQ_x = -S^\dagger K_x dS - dS^\dagger K_x S, \quad (\text{F5})$$

where we have used $K_x^{\text{in}} = K_x^{\text{out}} \equiv K_x$. To compute dS , we employ a newly introduced technique from Ref. [39]. First, we define another GWS operator Q_n , where our α parameter is now n , the index of refraction. We then have

$$Q_n = -iS^\dagger \frac{dS}{dn}. \quad (\text{F6})$$

Substituting this new operator into Eq. (F5), we get

$$\frac{dQ_x}{dn} = i(Q_n S^\dagger K_x S - S^\dagger K_x S Q_n), \quad (\text{F7})$$

which we can then take the expectation value of the $\vec{u}_{\text{max}}$ eigenstate to get the gradient of this eigenvalue, following Eq. (F4). Why does introducing another operator, Q_n , for each design pixel for which we want to change the refractive index, help us in computing the gradient of q_x with respect to the refractive index of all design pixels? Reference [39] shows that the elements of Q_n can be computed as

$$[Q_n]_{ij} = k^2 n \int_{\text{pixel}} \psi_i^*(\mathbf{r}) \psi_j(\mathbf{r}) dA, \quad (\text{F8})$$

where the integral is taking over the area of the design pixel, of which we want to compute $\partial_n q_x$, and $\psi_i(\mathbf{r})$ is the wavefunction resulting from an injection of the i th mode. Once the wavefunction $\psi_i(\mathbf{r})$ for every mode is computed, we can calculate the integral of Eq. (F8) for every design pixel without requiring the costly solving of the Helmholtz equation.

It should be noted, however, that this gradient is with respect to the *integrated* refractive index of each design pixel, but we want to be able to change the refractive index continuously across our optimization region. We eventually want to be able to see how q_x^{max} reacts to a change in refractive index in a single pixel of our design region, so we will instead limit our integral to a very small square of this region with area $\Delta x \Delta y$. Over this region, the integral is approximately $|\psi_u(\mathbf{r})|^2 k^2 n(\mathbf{r}) \Delta x \Delta y$, so we can see that the correct weight factor needed to see how q_x^{max} changes when n is changed over a small area is $k^2 n(\mathbf{r}) \Delta x \Delta y$. Putting this all together, we get the final local gradient of our cost function as

$$\frac{dq_x^{\text{max}}}{dn}(\mathbf{r}) = \vec{u}_{\text{max}}^\dagger \frac{dQ_x}{dn} \vec{u}_{\text{max}} k^2 n(\mathbf{r}) \Delta x \Delta y. \quad (\text{F9})$$

We now have a cost function (the largest eigenvalue of Q_x) and its gradient to optimize with. Our optimization is actually twofold with every iteration in gradient descent: First, we need to compute the eigenspectrum of Q_x and choose the largest eigenvalue, q_x . By doing so, we optimize the incoming wavefront by selecting the mode with the greatest pulling force. Then, we perform the main gradient descent optimization by minimizing this eigenvalue with respect to the refractive-index distribution of our design region. This makes it so that the *strongest possible* pulling force is minimized, so a more general superposition of eigenmodes will have an even weaker pulling force. This concludes our discussion on the pulling force operator Q_x , but we are not limited to just looking at the momentum transfer when working in the GWS operator framework.

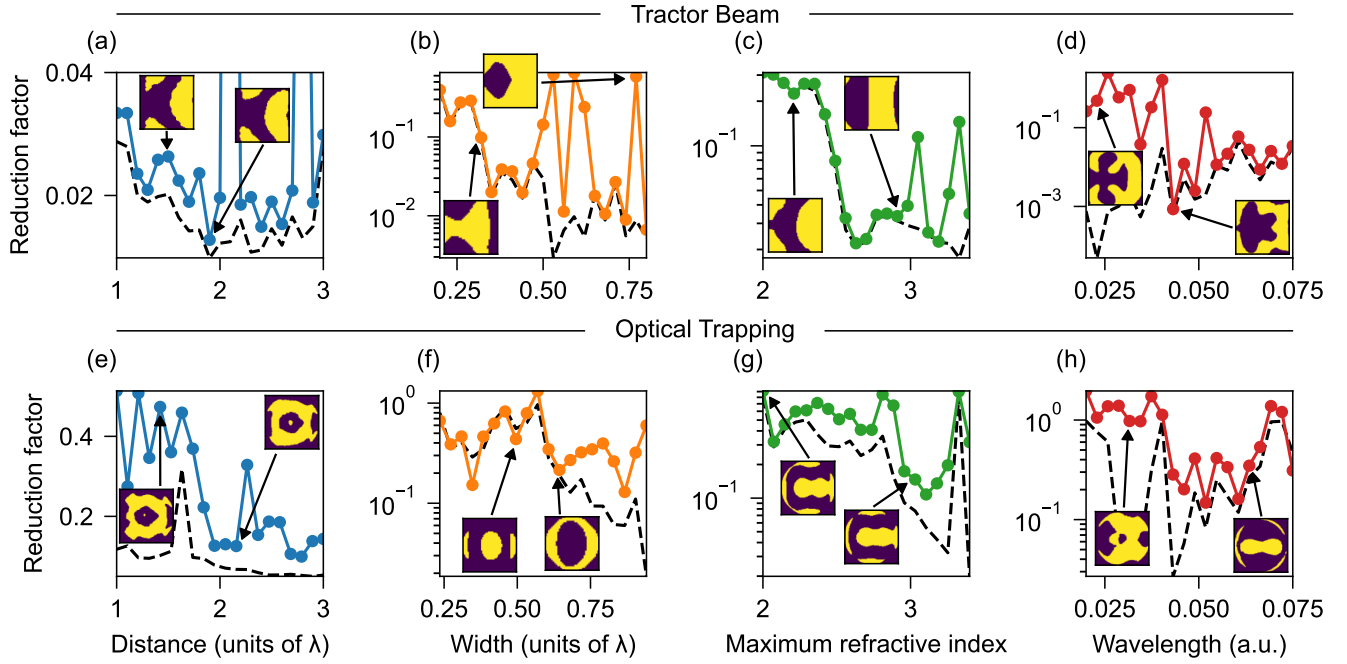


FIG. 10. Parameter sweeps with smoothing filter applied. The solid lines show by how much the optimal micromanipulation has been reduced for an inverse-designed target compared to a conventional structure with a uniform refractive index after the smoothing filter has been applied. The dashed lines show the reduction ratios for the original, unsmoothed structure (the same curves as Fig. 2).

2. Optical trapping stiffness micromanipulation

The most widely used method for manipulating objects with light is optical trapping. Trapping stiffness in the x direction is defined as $-\partial_x F_x$, so we define an operator W_x that computes the trapping stiffness for an arbitrary incoming wavefront as

$$W_x \equiv -\partial_x Q_x = i(S^\dagger K_x S K_x - K_x S^\dagger K_x S) = i[S^\dagger K_x S, K_x], \quad (\text{F10})$$

where $[\cdot, \cdot]$ denotes the commutator of two matrices. Again, we define the cost as the largest eigenvalue $w_x^{\max}$ and use Eq. (F10) to compute the derivative of W_x :

$$\frac{dW_x}{dn} = \left[\frac{d}{dn} (S^\dagger K_x S), K_x \right] = [[Q_n, S^\dagger K_x S], K_x], \quad (\text{F11})$$

where we have used the fact that K_x is independent of n . Now, the gradient computation follows a similar pattern as for Q_x and is given by

$$\frac{dw_x^{\max}}{dn}(\mathbf{r}) = \bar{v}_{\max}^\dagger \frac{dW_x}{dn} \bar{v}_{\max} k^2 n(\mathbf{r}) \Delta x \Delta y, \quad (\text{F12})$$

where $\bar{v}_{\max}$ is the eigenvector of W_x with the largest trapping stiffness.

We employ the same strategy as we did for the q_x optimizations. First, we create a randomized structure, compute the eigenvalues of W_x , and then minimize the largest eigenvalue with respect to the refractive-index distribution while varying the same parameters as before, with one major difference being that we restricted our design region to a circle instead of a square both to highlight the flexibility of our manipulation process and to connect to optical trapping experiments. It should be noted, however, that the maximal eigenstates $\bar{v}_{\max}$ of W_x do not necessarily result in a stable

trapping state. To ensure that the target is stably trapped, we find the appropriate wavestate $\bar{v}$ by considering the following optimization problem:

$$\max_{\bar{v} \in \mathbb{C}^n} \bar{v}^\dagger W_x \bar{v}, \quad (\text{F13})$$

$$\text{such that } \bar{v}^\dagger Q_x \bar{v} = 0, \quad (\text{F14})$$

$$\bar{v}^\dagger \bar{v} = 1, \quad (\text{F15})$$

This ensures that the force acting on the target is zero at the equilibrium position and that the wavefront is normalized.

APPENDIX G: COMPUTATIONAL DETAILS

1. Binarization and regularization

To create more fabricable structures that only consist of two materials, we use the technique of hyperbolic-tangent regularization, where the design region is parametrized by the new regularization variable $t \in (-\infty, \infty)$, instead of directly by the refractive index:

$$t(n) = \frac{1}{\beta} \operatorname{arctanh} \left(\frac{2(n - n_{\min})}{n_{\max} - n_{\min}} - 1 \right), \quad (\text{G1})$$

where $\beta > 1$ is a parameter that determines how steep the binarization is. We optimize with this t parameter, and then use the inverse relation to get back to our refractive-index distribution after the inverse-designed structure is complete:

$$n(t) = \frac{(n_{\max} - n_{\min})}{2} (\tanh(\beta t) + 1) + n_{\min}. \quad (\text{G2})$$

Following the chain rule, the gradient must be multiplied by a new factor:

$$\frac{dn}{dt} = \frac{\beta(n_{\max} - n_{\min})}{2 \cosh^2(\beta t)}. \quad (\text{G3})$$

TABLE I. Parameters used in Fig. 2. The width default for both trapping and tractor beam cases is 0.04 a.u. for the wavelength scans and is given below for all other scans.

Parameter	Defaults (tractor beam, trapping)	Range (tractor beam)	Range (trapping)
Wavelength λ (a.u.)	(0.05, 0.0425)	[0.025, 0.075]	[0.02, 0.075]
Refractive index $n_{\max}$	(3.0, 3.0)	[2.0, 3.4]	[2.0, 3.4]
Width ℓ (a.u.)	(0.02, 0.0325)	[0.01, 0.04]	[0.01, 0.0384]
Distance d (a.u.)	(0.05, 0.1)	[0.05, 0.15]	[0.05, 0.15]

The procedure is then to start with a randomized t distribution (rather than a randomized refractive-index distribution), convert it to a refractive-index distribution using Eq. (G2), and perform standard gradient-based optimization. Then, β is increased by a factor of 1.07 after every ten iterations of gradient descent, which forces the t distribution toward ± 1 . When we perform the gradient descent optimization while increasing β in this way, the cost function is incentivized to pick structures with a refractive index close to $n_{\min}$ or $n_{\max}$. This can be seen from the derivative dn/dt , in which the rate of change is large near the midpoint of $(n_{\max} - n_{\min})/2$, but practically 0 near $n_{\max}$ and $n_{\min}$.

As seen in Figs. 11 and 12, some of the structures still appear grainy and pixelated even after optimizing for binarized structures. To address this, we also analyzed how the reduction ratio of structures changes when a secondary smoothing filter is applied. To this end, we convolve each structure's normalized permittivity density, $\rho(\mathbf{r}) = [n(\mathbf{r})^2 - n_{\min}^2]/(n_{\max}^2 - n_{\min}^2)$, with a conic spatial filter with a radius of 4 pixels, which imposes a maximum feature size on the structure. Then, the filtered density is rebinarized via a smooth Heaviside projection and converted back to a refractive-index distribution:

$$\tilde{\rho} = \frac{\tanh(\beta_{\text{proj}}\eta) + \tanh(\beta_{\text{proj}}(\rho - \eta))}{\tanh(\beta_{\text{proj}}\eta) + \tanh(\beta_{\text{proj}}(1 - \eta))}. \quad (\text{G4})$$

In our analysis, we used $\beta_{\text{proj}} = 2^{12}$ and $\eta = 0.5$. The full set of smoothed structures can be found in Figs. 13 and 14, and the reduction ratio parameter scans are shown in Fig. 10.

2. Parameter scans

We will now provide exact details about the nature of our gradient descent optimization for q_x and w_x when varying parameters of the system. We choose to normalize q_x and w_x by the eigenvalues computed for a conventional target to see how well the optimized structure performs when compared to

it and to make our cost functions dimensionless. In this paper, we chose a solid structure with a constant refractive-index distribution set to $n_{\max}$ everywhere as our baseline.

When varying a given parameter, we chose default values for the rest of the parameters that gave a good compromise between minimization performance and computation speed for both inverse-design procedures, with exact values found in Table I. Each parameter (except $n_{\max}$, which is dimensionless) is given in arbitrary units. In these units, the radius of the entire simulated region is $R = 0.1$, so a target in the center of the scattering region is at a distance of 0.1 from the wave's source. For all figures in the main paper, we gave λ in arbitrary units and the rest of the dimensionful parameters in units of the default value of λ .

To begin our numerical optimization, we partitioned the region into discrete pixels (in this paper, the density was 22 500 pixels per wavelength squared). Next, a structure with a randomized refractive index was generated, and the cost function was defined as the ratio of this new structure's most positive eigenvalue to that of the base result. Using this randomized refractive-index distribution as an initial guess, gradient descent was performed on the cost function using the SLSQP algorithm.

Logically, setting up the optimization in this way often results in trivial structures, where all pixels are set to the refractive index of vacuum, i.e., resulting in no structure at all. To fix this, we implemented a constraint to our optimization based on the average “fill density” $\mathcal{D}$:

$$\mathcal{D} \equiv \left\langle \frac{n(\mathbf{r}) - n_{\min}}{n_{\max} - n_{\min}} \right\rangle, \quad (\text{G5})$$

where $\langle \cdot \rangle$ denotes averaging over the refractive index at every position in the design region. In this paper, we constrained our optimization such that $\mathcal{D} > 0.5$; i.e., any structure generated must be at least “half-full” on average.

APPENDIX H: EXTENDED DATA FIGURES

Here, we present the full dataset of inverse designed structures underlying this work.

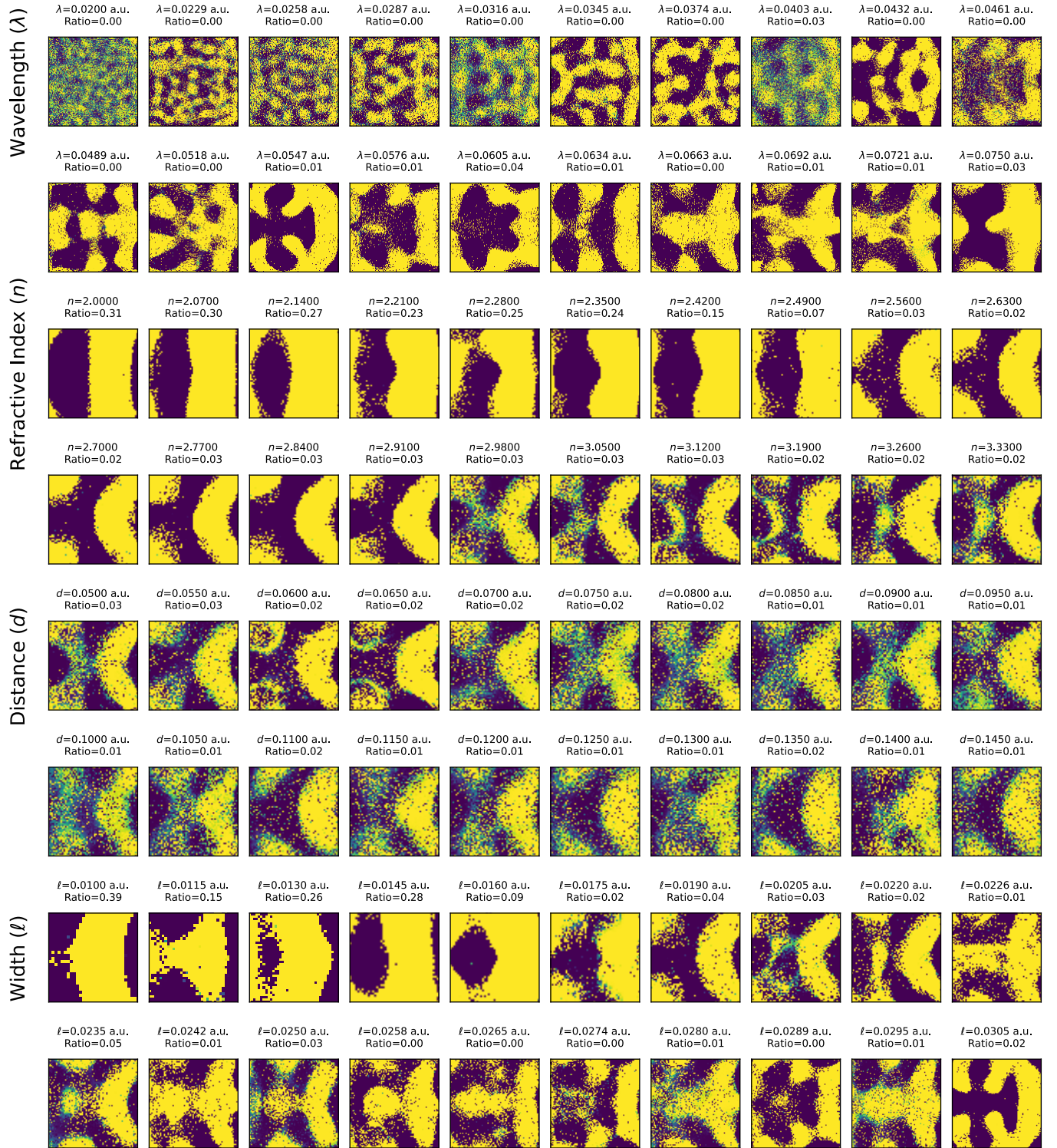


FIG. 11. Tractor beam minimizing structures. Plots show all structures used in Figs. 2(a)–2(d), with parameters given in arbitrary units. These structures were all generated using tanh regularization to minimize $q_x^{\max}$. The reduction factor (“ratio”) of the optimal pulling force compared to the conventional structures is also given.

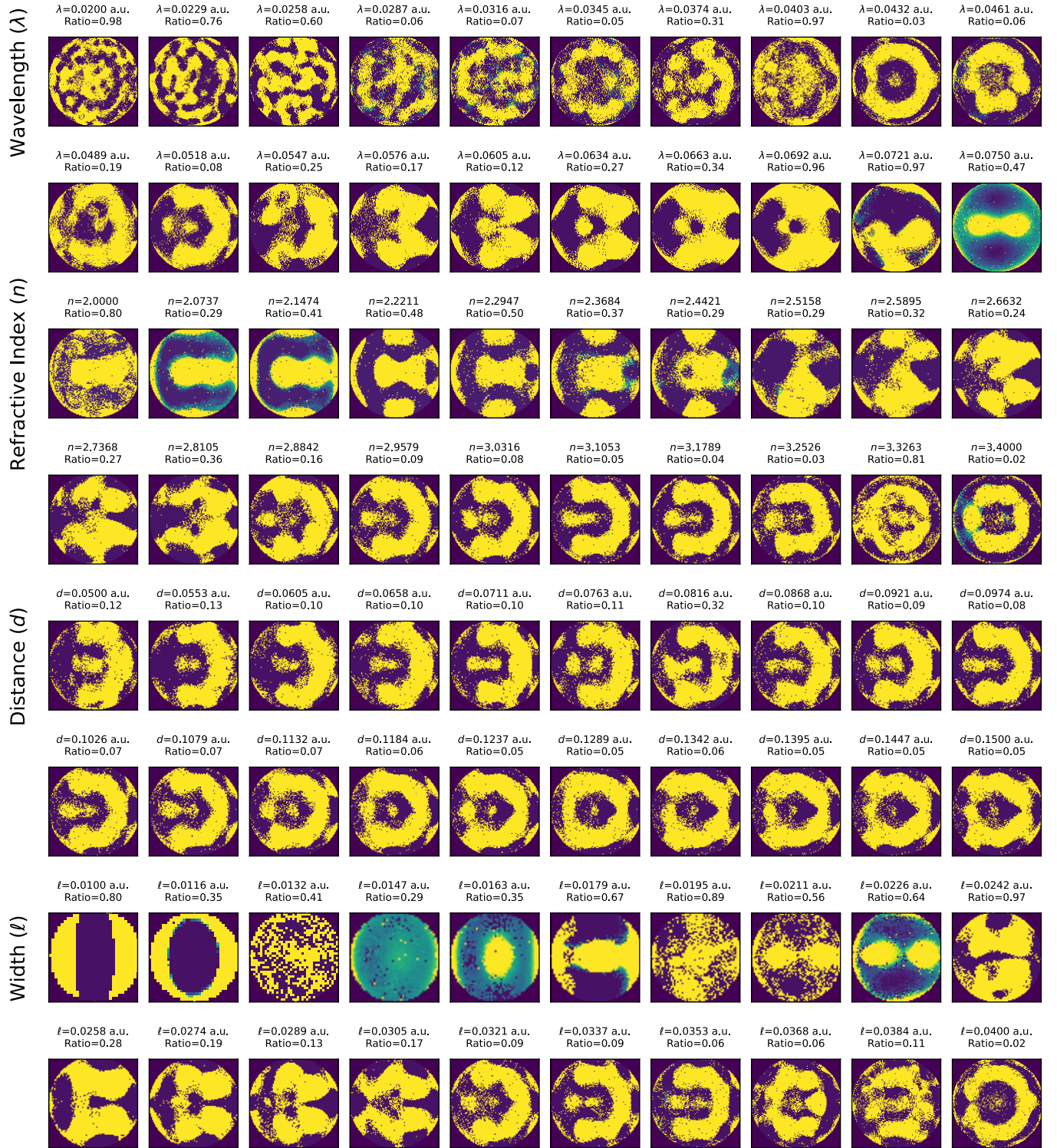


FIG. 12. Trapping stiffness minimizing structures. Plots show all structures used in Figs. 2(e)–2(h), with parameters given in arbitrary units. These structures were all generated using tanh regularization to minimize $w_x^{\max}$. The reduction factor (“ratio”) of the optimal trapping stiffness compared to the conventional structures is also given.

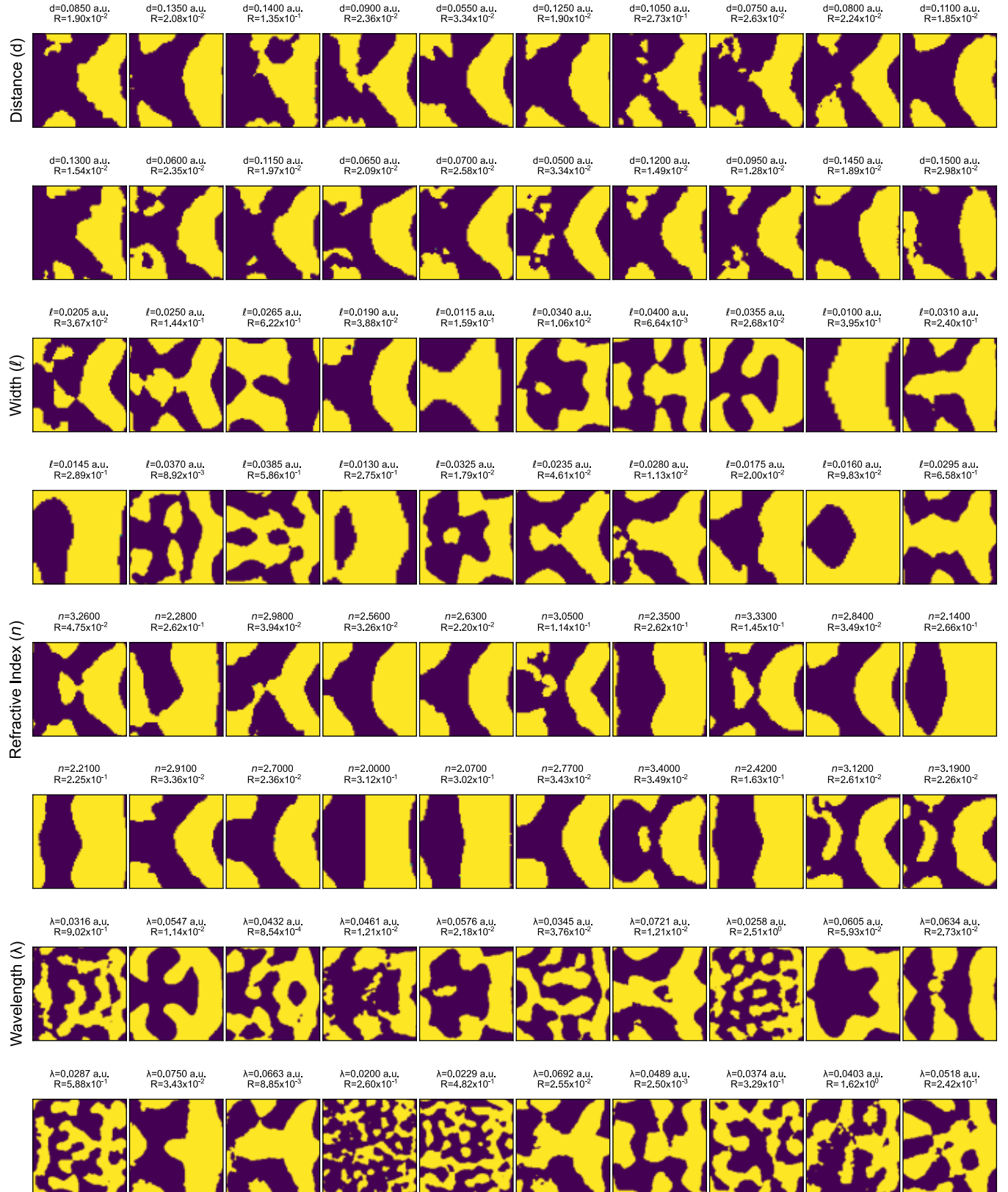


FIG. 13. Tractor beam minimizing structures with Gaussian smoothing applied. Plots show all structures from Fig. 11 after the smoothing filter has been applied. The updated reduction ratios are also given.

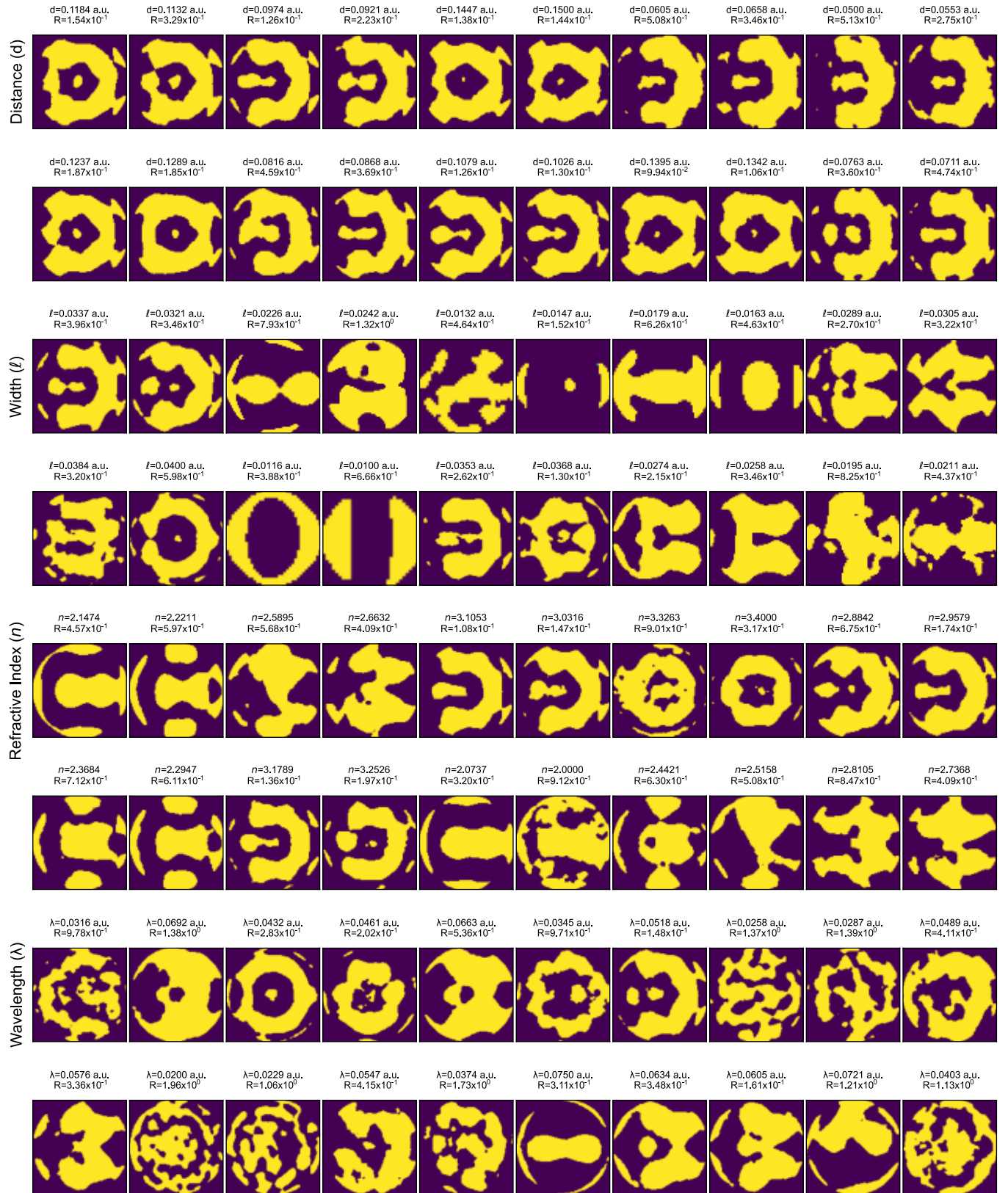


FIG. 14. Trapping stiffness minimizing structures with Gaussian smoothing applied. Plots show all structures from Fig. 12 after the smoothing filter has been applied. The updated reduction ratios are also given.

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