Research Article

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Accounting for laser beam characteristics in the design of freeform optics for laser material processing

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Abstract: Recently, freeform optics have been introduced for application adapted beam shaping in laser heat treatment. There, intensity distributions are generated that induce previously defined temporal and spatial temperature profiles. To this end, a two-step simulation strategy is necessary, where in the first step the intensity distribution must be derived for which in the second step the freeform optics is calculated. To provide a design that can successfully be integrated in an experimental setup, the incoming laser beam's characteristics must be accounted for in the derivation of the adapted intensity distribution as well as in the freeform optics design. Here, the two most relevant quantities are the beam's maximum output power as well as the divergence angle. In this work, strategies are presented that account for the beam's maximum output power in the derivation of the adapted intensity distribution. Furthermore, stabilizing methods are introduced to enhance the performance of a previously introduced freeform optics design algorithm that takes into account the laser beam's finite divergence angle but suffers from numerical noise and oscillation problems. A simulation example that uses both techniques is given for (nano) ceramic thin-film laser processing.

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1 Introduction

For many years now, freeform optics have been showing to be a very powerful tool in illumination optics for different applications such as automotive, streetlight, or general illumination [1–3]. More recently, publications relating to freeform optics have also been focusing on laser beam shaping for material processing [4, 5]. Because of their high number of degree of freedoms, they especially enable the generation of intensity distributions that are specifically adapted to the particular laser processing application. (In this work, light distributions are presented in units of energy per area, which in the context of laser technology is usually referred to as 'intensity', whereas for radiometry the same quantity is called 'irradiance'. As this paper deals with applications for laser material processing, the term 'intensity' is preferred and used throughout this paper.) One such task – in laser heat treatment applications – is to form the intensity distribution so that a previously defined spatial and temporal temperature profile is induced within the processed workpiece [6]. These intensity distributions usually are very inhomogeneous so that conventional beam shaping strategies based on spherical or aspherical optics do not provide enough design freedom.

For the derivation of such application adapted intensity distributions, a preliminary simulation step is necessary to calculate the corresponding intensity distribution from the prescribed temperature profile. It has been shown that this problem can be formulated as an inverse heat conduction problem that is solved using optimization strategies [7, 8]. The approach has been verified for applications such as laser hardening, laser softening, laser thin-film processing, or laser-assisted tape placement [5, 9, 10].

For experimental validation, it is necessary to account for the incoming laser beam's properties such as the finite laser power, the intensity distribution, and the finite

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divergence angle. Although the finite laser power must be considered when deriving the necessary intensity distribution, the beam's intensity distribution and the finite divergence angle must be taken into account when designing the freeform optics.

In Ref. [8], the finite laser power is respected in the solution of the inverse heat conduction problem through some trial-and-error approach. The input parameters are guessed and it is then checked if the space integral over the intensity lies below the available laser power. If this is not the case, the process parameters are adapted manually. This is iterated until a satisfactory result is obtained. This, however, is neither an elegant nor an efficient approach.

Although, in general, every freeform optics design algorithm respects the incoming intensity distribution, it has proven to be challenging to respect the beam's finite divergence angle, which corresponds to respecting the finite étendue of the source. Here, two main approaches have been suggested. The first one is based on iteratively adapting the target distribution and calculating the freeform optics, assuming perfect collimation [11–13]. This yields satisfactory results only in cases where the étendue is not too high. The other approach is based on the mathematical optimization of the freeform optics, whereas the calculation of the intensity distribution that is generated with a given optics is performed for the 'real' light source [11, 14, 15]. Several approaches to efficiently perform this calculation have been described. Although this approach is, in general, applicable, it is often subject to numerical issues and oscillations arise [15]. Furthermore, the optimization usually converges to local minima only.

In this work, an exemplary case is considered in which a steel sheet is being treated for the coating with (nano) ceramic thin films for wear protection. It has been shown that, for this application, laser-based processes enable the coating on temperature-sensitive substrates, which is not achievable with conventional oven-based techniques [16]. In the following, an adapted laser beam intensity distribution shall be derived that, for a constant feed speed, generates a stepped temperature profile within the irradiated area. This temperature profile aims at combining two processing steps – drying and curing – which usually require very different temperatures into a single processing step. In this way, an increase in the efficiency of the overall treatment is obtained as only a single laser processing step is necessary. In a previous work [17], a comparable intensity distribution has been derived but the laser beam characteristics have not been accounted for in the design algorithms themselves. Now, the size of the irradiated area should be as large as possible and it should only be restricted by the maximum laser power that is supposed to be 800 W. Furthermore, the intensity distribution and the divergence angle of the laser beam have been measured so that the freeform optics shall be designed accordingly. While the intensity distribution follows a super-Gaussian-like shape, the divergence angle lies at 2.44 mrad.

Thus, the approaches described in the literature must be extended with regard to two aspects. First, the solution of the inverse heat conduction problem is enhanced so that the spatial extent of the intensity distribution is automatically determined, taking into account the given maximum available laser power. Furthermore, stabilization strategies are implemented in the freeform optics design algorithm for nonzero étendue sources.

The paper is structured as follows. Section 2 describes the simulation methods. There, a short summary of the two principal algorithms – one for the solution of the inverse heat conduction problem and one for the design of the freeform optics – is provided. Furthermore, the adaptations to the two problems stated above are described. Section 3 then follows with simulation results for the given situation before the work concludes with a summary and an outlook.

2 Simulation methods

In this section, the algorithms, as described in the literature, are summarized and the extensions to the given problem are presented.

2.1 Solution of the inverse heat conduction problem

A laser beam that is moving at constant feed speed $\vec{v}$ over the surface of a workpiece is inducing a temperature profile T that will after a while reach a steady state. This steady-state temperature profile can be calculated using the heat conduction equation [18]:

$$-\nabla(k(T)\nabla T) = s - \vec{v}\rho(T)c_p(T)\nabla T$$

where $k(T)$ refers to the heat conductivity, $\rho(T)$ refers to the mass density, and $c_p(T)$ refers to the specific heat at constant pressure. The absorbed intensity I is either included in the source term s (for volume absorption) or as surface flux in a Neumann boundary condition of the form $-k\vec{n}\nabla T = A\cdot I$ (for surface absorption) with the boundary normal $\vec{n}$ and the absorptivity A. Additionally, boundary conditions need to be specified for every (other) boundary of the workpiece.

This is the usual approach for calculating the temperature profile for a given intensity distribution, which in the given context is called the solution of the 'direct' heat conduction problem. The corresponding 'inverse' heat conduction problem is then defined as follows [19]: given the information of the temperature profile, the intensity distribution must be reconstructed. Although the direct heat conduction problem can be solved with standard solution strategies for partial differential equations [finite difference method (FDM) and finite element method (FEM)], the inverse heat conduction problem is known to be ill-posed and special regularization strategies must be implemented.

The presented solution strategy for the inverse heat conduction problem is based on the conjugate gradient method with adjoint problem [20, 21].

In this approach, the temperature is assumed to be prescribed on a set of N points, which are located somewhere within the workpiece or on its surface. It is then possible to qualify a given intensity distribution by comparing, at these points, the temperature it induces with the prescribed temperature through calculating the least-squares sum

$$S=\sum_{i=1}^{N}(Y_i-T(\vec{r}_i))^2$$

Here, Y_i is the prescribed temperature at point $\vec{r}_i$ and $T(\vec{r}_i)$ is the calculated one.

This least-squares sum is minimized iteratively. In each iteration, the intensity distribution is updated according to the instruction

$$I^{n+1}=I^n-\beta^n d^n$$

Here, d^n is the actual update direction that is given as a combination of the previous update direction and the steepest decent direction given by the gradient of S with respect to the intensity distribution, i.e. ∇S_I.

$$d^n=\gamma^n d^{n-1}+\nabla S_I^n$$

β^n and γ^n are real numbers that are called step size and conjugation coefficient, respectively.

The computation of the different quantities – ∇S_I^n, β^n, γ^n – is rather comprehensive and includes the solution of two further partial differential equations: the adjoint problem and the sensitivity problem.

In the conjugate gradient method with adjoint problem, a regularized solution is obtained by limiting the number of iterations. See Refs. [7, 8] for more information.

2.2 Spot size optimization

This algorithm, as described above, is applicable in a situation where the intensity distribution's dimensions are well specified. However, for great dimensions, it might yield results that are not realizable as the total power needed is higher than the available maximum laser power. In such a case, the intensity's dimensions must be decreased and the prescribed temperature profile must be adapted where necessary. Furthermore, in cases where the temperature profile is prescribed through a temperature-time-development, the feed speed must also be adjusted.

Here, it is suggested to adapt the intensity distribution's dimensions iteratively according to

$$D^k=D^{k-1}\cdot\sqrt{\min\left(0.99, c\cdot\frac{P_{\mathrm{max}}}{P_{\mathrm{actual}}}\right)}=D^{k-1}\cdot f$$

where D is the size in the x- and y-directions, respectively, P_{max} is the maximum available laser power, P_{actual} is the needed power in the last iteration, and c is a factor (usually chosen between 1 and 2). This factor c accounts for the fact that the needed power does not scale linearly with the extent and shall slow down the convergence.

In the implementation, the spot size reduction is performed for an equally spaced intensity with a previously defined discretization size δ. Thus, D^k is chosen as

$$D^k=\delta\cdot\mathrm{floor}\ (n_D^{k-1}\cdot f-1)$$

with n_D^{k-1} being the number of points in the previous iteration.

In cases where the temperature profile is prescribed as 'within the irradiated area', the points with prescribed temperature values can be adjusted via

$$p^k=p^{k-1}\cdot\frac{D^{k-1}}{D^k}$$

where, for p, the points' x and y-coordinates must be inserted. An analogous relation holds for a possible adaptation of the feed speed.

2.3 Freeform optics design strategy

The freeform design algorithm [15] is based on calculating the intensity distribution generated by a given freeform optics at a target point (x_t, y_t) on the target surface by integrating the incoming light [11]:

$$\begin{aligned}E(x_t, y_t)&=\int L(x_t, y_t, \phi_t, \theta_t)\cos\theta_t d\Omega_t\\&=\int L(x_t, y_t, \phi_t, \theta_t)\cos\theta_t\sin\theta_t d\theta_t d\phi_t\end{aligned}$$

Here, $E(x_t, y_t)$ is the intensity at position (x_t, y_t) and $L(x_t, y_t, \phi_t, \theta_t)$ is the radiance at position (x_t, y_t) propagating into the direction given by (ϕ_t, θ_t). The index t refers to coordinates in the target plane.

The integrals over the solid angles are then approximated by sums and a single ray is associated with every single entry. As the radiance stays constant, when a ray propagates through any optical systems (as long as Fresnel losses are neglected), it is then possible to insert the ray's radiance in the source plane, i.e.

$$\begin{aligned} E(x_t, y_t) &= \sum_{j=1}^{N_{\text{rays}}} L(x_{t,j}, y_{t,j}, \phi_{t,j}, \theta_{t,j}) \cos\theta_{t,j} \sin\theta_{t,j} \Delta\theta_{t,j} \Delta\phi_{t,j} \\ &= \sum_{j=1}^{N_{\text{rays}}} L(x_{s,j}, y_{s,j}, \phi_{s,j}, \theta_{s,j}) \cos\theta_{t,j} \sin\theta_{t,j} \Delta\theta_{t,j} \Delta\phi_{t,j} \end{aligned}$$

Thus, the intensity on the target plane can be calculated by considering rays emitted from the target plane and traced backward through the system. If they intersect the source, the radiance is evaluated and the according term is added to the sum.

In this setup, the optical surfaces are assumed to be B-splines that have several advantages; the most important one is that they enable a continuous parameterization. The degrees of freedom are currently given by the control points' z-components.

This calculation of the intensity distribution is then combined with a standard optimization strategy, which is, as before, based on a least-squares sum. This time, the current intensity distribution is compared to the target intensity distribution on a set of target points.

$$S = \sum_{i=0}^{N_{\text{points}}} (E_{\text{actual}}(x_{t,i}, y_{t,i}) - E_{\text{target}}(x_{t,i}, y_{t,i}))^2$$

2.4 Stabilization

This algorithm, as described in Ref. [15], yields freeform optics that are in principle satisfactory. However, the surfaces of the freeform optics exhibit many oscillations that are due to numerical issues. Furthermore, irregularities also appear in the obtained target intensity distribution, which arise from the impossibility to obtain sharp transitions between darker and brighter areas. On the one hand, this holds for edges at the boundary of the target; on the other hand, it also influences edges (i.e. sharp lines) in the inner part of the target distribution.

Therefore, the algorithm is extended to stabilize it. There are two main extensions:

a. Refinement: Some refinement strategy has been implemented that iteratively increases the number of degrees of freedom of the freeform surfaces. At the beginning, an initial design is calculated with only ≤100 degrees of freedom. When the optimization converges, the number of degrees of freedom is increased by a factor that usually lies between 1 and 4. With this, the optics is recalculated and the procedure is repeated several (usually up to five) times leading to ≥1000 degrees of freedom in the final design.

b. Smoothing of target distribution: In the second extension, the target intensity distribution is adapted to account for the finite étendue of the laser beam. This assures that the target intensity distribution is achievable, at least in principle.

The following considerations are based on the concept of étendue, which is defined differentially as [22]

$$dU = n^2 dA \cos\theta \, d\Omega$$

Here, a ray bundle with solid angle $d\Omega$ is considered to pass through a differential surface area dA, whereas the angle between the bundle's propagation direction and the surface normal is given by θ. The surrounding material is supposed to have the index of refraction given by n. The étendue can thus be depicted as a measure for the light's extension in space and angle, i.e. the volume it occupies in phase-space.

It has been proven that the étendue stays constant when the light propagates through an optical system (no scattering assumed). Thus, there will also be some impact on the achievable target intensity distribution, which especially results in the broadening of sharp edges. An estimation for the minimum width of any edge can be obtained by equalizing the étendue of the source to that in the target plane. Supposing that both source and target are surrounded by air, it holds

$$U_s = U_t \Leftrightarrow \int dA_s \cos\theta_s d\Omega_s = \int dA_t \cos\theta_t d\Omega_t$$

As only an approximation for the width of the edge shall be provided, it is possible to assume that the emittance angle of a ray does not depend on its position on the source and that, furthermore, the maximum angle under which rays impact on the target plane does not depend on the target position. It is then possible to derive

$$A_s(\sin\theta_{s,\max})^2 = A_t(\sin\theta_{t,\max})^2$$

where $\theta_{S,\max}$ is the source divergence angle, A_s is the source size, and $\theta_{t,\max}$ is the maximum angle under which rays impact on the target plane. Then, A_t is the minimal area on which the light can be concentrated. The minimal width of the edge can thus be determined by calculating

$$d_t \approx \frac{\sin \theta_{s,\max}}{\sin \theta_{t,\max}} \sqrt{A_s}$$

Before starting the optimization, the target intensity distribution is smoothed until every edge is approximately broadened to that size. With this, the algorithm proves to converge more reliably.

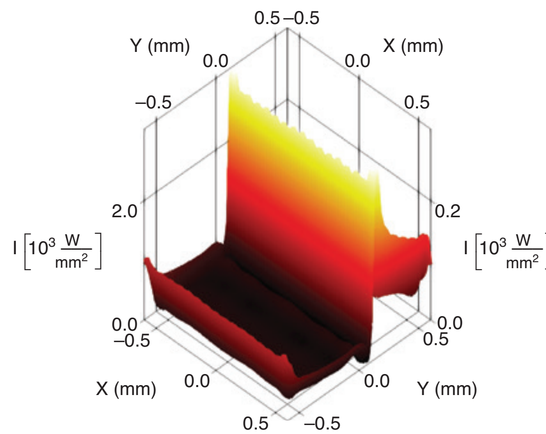

Figure 1: Calculated intensity distribution.

3 Results

In the first part of this section, the results for the calculated intensity distribution are presented. Afterwards, the design of the freeform optics is shown.

3.1 Derivation of the intensity distribution

As stated in Section 1, the aim is to calculate an intensity distribution for a laser thin-film processing application that induces a stepped temperature distribution of 400°C and 1500°C, respectively, within the (rectangular) area irradiated by the laser beam. To this end, a steel sheet with dimensions of $4\times4\times1$ mm^3 is assumed over whose z-surface the laser beam is initially moving with $v_y = -500$ mm/s. As the penetration depth of light in the visible and infrared wavelength range in steel is very low, the absorption of the laser radiation is simulated as a surface flux, i.e. through a Neumann boundary condition. Furthermore, the boundary condition $T=20$°C is applied to the boundary at $y=-2$ mm and the other boundaries are supposed to be adiabatic.

Start dimensions of 2×2 mm^2 are chosen for the intensity distribution and the procedure from Section 2.2 is applied to compute an intensity distribution for which the total power lies below 800 W. Additionally, as the prescribed temperature profile is given as a temperature-time-profile, the feed speed is adapted to the spot size so that the total irradiance time stays constant.

This approach then yields an intensity distribution with an extent of 1.2×1.2 mm^2, as shown in Figure 1. The total power is 778 W, which lies well below 800 W. It consists for each temperature step of three thin lines with high-intensity values at the edges of the corresponding area. The rest of the intensity distribution is rather flat.

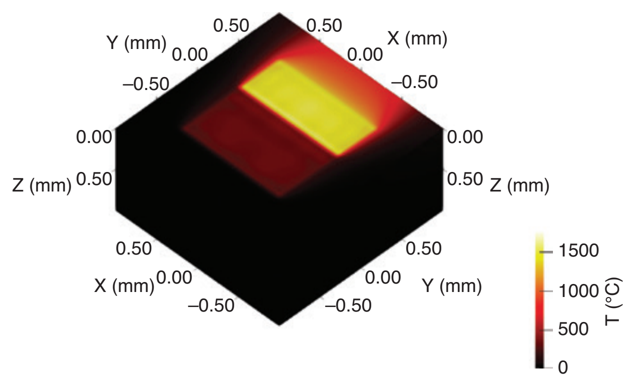

Figure 2: Temperature profile that has been obtained with the intensity distribution in Figure 1.

There are small oscillations visible at the sharp edges of the intensity distribution, which are due to mapping issues of the N points with prescribed temperature to the FDM mesh vertices. However, they can be neglected as the intensity distribution will be smoothed in Section 3.2 anyway.

The temperature distribution that is calculated (for a smaller volume) using this intensity distribution is shown in Figure 2. The two different temperature steps are clearly distinguishable and well-defined and the temperature is very homogeneous in each step. This temperature distribution has been obtained using the commercial FEM software ANSYS [23] and thus provides a validation for the computed intensity distribution.

3.2 Freeform optics design

The intensity distribution shown in Figure 1 has a rather small extent and very sharp features. The geometry that

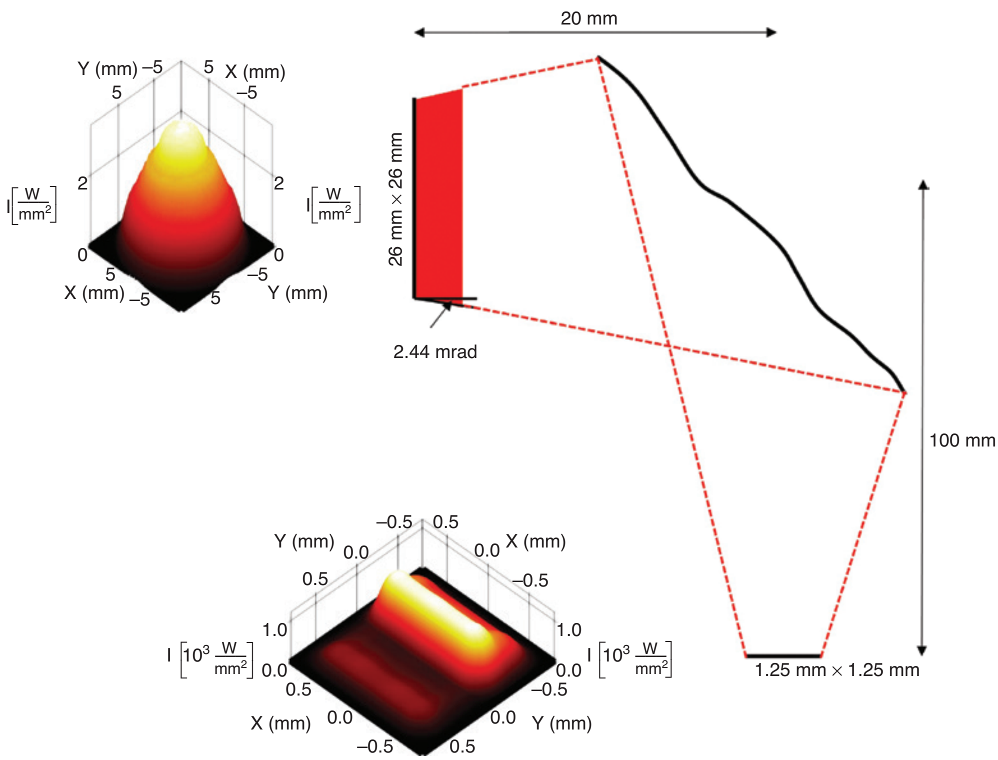

Figure 3: Geometrical setup for the freeform optics design showing also the input and prescribed intensity distributions.

is assumed for the experimental setup is depicted in Figure 3. The laser beam with a super-Gaussian-like intensity distribution (it is taken from measurements) is incident on a freeform mirror, which changes the propagation direction by 90°. The working distance is assumed to be 100 mm. Figure 3 also shows the measured input intensity and the (smoothed) target intensity.

According to the approximate relation given in Section 2.4, the minimum achievable edge width can be estimated to be 0.3 mm. As this is a significant fraction of the intensity's general size, it is not possible to neglect effects due to the finite divergence angle. Thus, it is not possible to apply an algorithm assuming zero étendue light.

Therefore, the algorithm described in Section 2.3 is implemented and the target intensity is smoothed as shown in Figure 3. As an initial guess, a parabolic surface is assumed with 49 degrees of freedom. The target intensity distribution is prescribed on 151×151 equally spaced points on the target plane. The source intensity measurement is interpolated on 400×400 positions and the angular spectrum of the source is assumed to be Gaussian with a divergence angle of 2.44 mrad. The freeform mirror is refined three times leading to 1225 degrees of freedom in the final setup.

The obtained intensity distribution is simulated using the ray tracing software ZEMAX [24] and the result is shown in Figure 4. It is very close to the prescribed (smoothed) intensity distribution in Figure 3, although there is, of course, some deviation to the initial intensity distribution in Figure 1 due to the finite étendue and the smoothing.

The mirror design is shown in Figure 5 where the small overall curvature arises as a light beam with a diameter 26 mm is focused to a much smaller extent. It is furthermore obvious that the surface and the achieved intensity are quite smooth and that they show much less irregularities and oscillations as for similar situations in our previous publication [15].

As a final check, it is possible to evaluate the temperature profile that is obtained with the intensity distribution

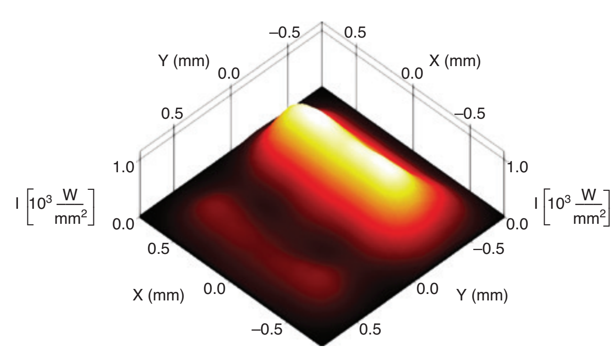

Figure 4: Obtained intensity distribution.

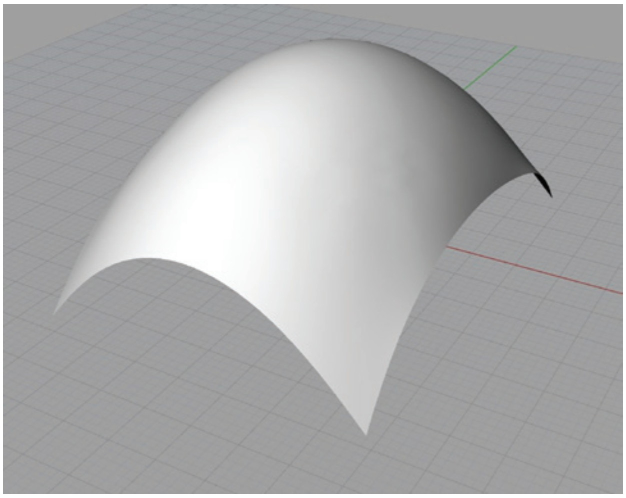

Figure 5: Freeform optics design scaled by a factor of 10 in the direction of the overall surface normal.

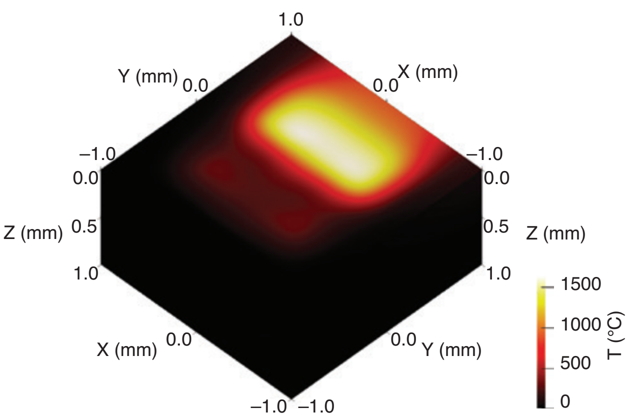

Figure 6: Calculated temperature profile for the intensity distribution shown in Figure 4.

in Figure 4. Figure 6 shows the result. It is obvious that the effect of the finite divergence angle is recognizable and that there is a difference between the temperature distributions in Figures 2 and 6, respectively. Most prominently, the sharp edges at the boundary of the laser spot as well as the edge between the lower and the upper temperature step are broadened. This had to be expected as the intensity distribution is broadened likewise by the finite étendue. However, the temperature profile is supposed to agree sufficiently with the requirement, as the different temperature steps are clearly distinguishable.

4 Conclusion and outlook

This work contributes to the design of freeform optics for laser material processing where the laser beam's intensity distribution is formed to induce application-specific temporal and spatial temperature profiles in the workpiece. The focus lies on respecting the constraints that are inherent to the task because of the characteristics of the input laser beam. Here, strategies are described that respect the maximum output power in the derivation of the necessary intensity distribution and account for finite divergence angles in the freeform optics design. For the latter, methods are described that stabilize an existing algorithm.

The performance of the presented approach is shown using an example from thin-film laser processing where the input laser beam's characteristics have been accounted for. The size of the intensity distribution is adapted to the maximum output power and the freeform optics is designed respecting the finite divergence angle. It is furthermore shown that the achieved temperature profile agrees suitably with the specifications.

For the freeform optics design, a method has been introduced that transforms the prescribed intensity distribution in such a way that the new target intensity distribution is in fact physically achievable with the 'real' laser beam. This stabilizes the mathematical optimization. In the considerations leading to an approximation for the minimal edge width, it was assumed that the maximum incident angle of the light does not vary with the position on the target. This simplification is probably too wide in many cases of interest and results can be improved by considering a spatially variant approach. Here, a more detailed consideration is supposed to produce target intensity distributions that are closer to the original (prescribed) one.

Moreover, the presented approach of stabilizing the freeform optics design algorithm through the smoothing of the target intensity distribution is only one approach of obtaining an intensity distribution that is physically achievable and acceptably close to the initial prescribed one. Further studies might focus on obtaining achievable smooth target intensity distributions with an increased agreement, e.g. by transforming the initial (unsmoothed) target intensity distributions into a different one before smoothing.

Concerning the thin-film processing application, future work will focus on the realization of the experimental setup. To this end, the designed freeform optics will be manufactured by diamond turning and afterward integrated in a laser processing test stand.

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Annika Völl studied physics at the RWTH Aachen University and KTH Stockholm with a focus on theoretical solid-state physics. Since 2014, she is working at the Chair for Technology of Optical Systems at the RWTH Aachen University, where she is actually pursuing her Ph.D. In her work, she is mainly focusing on freeform optics and application adapted laser beam shaping.

Rolf Wester
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Rolf Wester is a scientist at the Fraunhofer Institute for Laser Technology (ILT). He received his M.Sc. in physics in 1983 from the Technical University of Darmstadt and his Ph.D. in 1987 from the RWTH Aachen University. In the same year, he transferred from the RWTH Aachen University to the Fraunhofer ILT, where he gained a broad range of expertise among others in the fields of laser excitation, plasma physics, and thermomechanics. The main focus of his work during the last 20 years was on the field of optics including wave optics and nonlinear optics. Since about 8 years, he is working in the field of freeform optics.

Michael Berens
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Michael Berens is a researcher at the Chair for the Technology of Optical Systems at the RWTH Aachen University and has been working on methods for designing freeform surfaces with additional optical elements as well as using probabilistic methods to describe radiance distributions in optics design. Previously, he has graduated with a diploma in physics in 2012 from the RWTH Aachen University.

Paul Buske
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Paul Buske is studying physics at the RWTH Aachen University and UV Valencia since 2013 with a focus on quantum field theory and gauge theories. He started working as a student assistant at the Chair for Technology of Optical Systems at the RWTH Aachen University in 2015 and has recently begun to write his master thesis, which is related to freeform optics design for laser beam shaping.

Jochen Stollenwerk
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Jochen Stollenwerk studied physics at the RWTH Aachen University, with a focus on solid-state physics and laser technology from 1990 to 1996, after which he worked as a research associate at the Fraunhofer ILT in the field of laser material processing. In 2001, he received his doctorate in mechanical engineering from the RWTH Aachen University. From 2001 to 2004, he was a manager at the TRUMPF Laser Marking Systems, Switzerland. Since 2004, he is the vice director at the Chair for Technology of Optical Systems at the RWTH Aachen University. From 2004 to 2017, he also headed the research group ‘Thin Film Processing’ at the Fraunhofer ILT. Parallel to his work at the RWTH Aachen University, he now works in the field of innovation management at the Fraunhofer ILT.

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Peter Loosen studied physics at the Technical University Darmstadt where he graduated in 1980 in the field of lasers for industrial manufacturing. From 1980 to 1984, he was a scientific employee at the Institute of Applied Physics at TU Darmstadt. After he received his doctorate in 1984 in the area of ‘High-Power CO_2-Laser with Axial Gas Flow’ from TU Darmstadt, he transferred to the Fraunhofer ILT where he became responsible for the departments ‘Gaslaser’, ‘Solid-State Lasers’, ‘Metrology’, and ‘Plasma Systems’. Since 1993, he is the deputy head of Fraunhofer ILT; since 2004, he is a professor for ‘Technology of Optical Systems’ and the head of the newly formed respective chair at the RWTH Aachen University.