

Use of molecular dynamics method for dot pattern design of a thin light guide in an LED backlight

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Abstract. We propose a molecular dynamics method dot generation scheme incorporating the periodic boundary and fixed-cell boundary geometrical conditions to generate random dot distribution on the order of several million dots for use in the base of a thin light guide. In addition, the generation scheme can be used to easily adjust the dot density at any local region from illuminance causing feedback in the optical design phase. Based on the incorporation of these two geometrical conditions, the generation of the random dots for the whole LED light guide can be simplified to just three subdomains, one domain represented by the periodic boundary condition, and the other two domains represented by the fixed-cell boundary condition. Employing these conditions significantly shortens the computational time necessary to obtain optimal random dot distribution and subsequent optical optimization on a PC using optical commercial software. © 2009 Society of Photo-Optical Instrumentation Engineers. [DOI: 10.1117/1.3253682]

Subject terms: edge-lit backlight; light guide; random dot generation; molecular dynamics method; periodic boundary condition; fixed-cell boundary condition.

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1 Introduction

Due to improvements in the brightness of light emitting diodes (LEDs) in recent years,¹⁻⁴ the LED has become a more suitable candidate for a light source in midsize backlights such as notebook computers, automobile DVD players, and game systems such as Nintendo's Gameboy. The utilization of these LED light sources can significantly reduce the thickness of the light guide for extremely thin and lightweight backlight modules.⁵⁻⁹ However, if a thinner light guide is used, smaller-sized microstructures (or dots) must be used to create a smoother backlight field, as larger dots tend to produce a more "grainy" field, showing traces of individual microstructures. This increases the number of the dots necessary for use in the base of the light guide. For example, from a practical application perspective, for a typical 14-in notebook monitor, approximately 1.6 million dots are required at a dot diameter of 80 μm . If 50- μm dots are used, however, 4 million dots will be required to provide the same percentage of dot coverage. Thus, an efficient method to generate such a large number of dots is undoubtedly needed, as well as a dot pattern optimization method,

in order to reach the uniformity requirement, defined as the ratio between minimum and maximum luminance within the entire backlight.

There are two procedures constituting dot optimization in light guide design: the dot generation scheme and the optical design phase. Each dot pattern generated by the former scheme is simulated in the latter through numerous iterations that generate an optimal dot pattern in order to fulfill the uniformity requirement. A successful dot optimization scheme would be efficient in terms of design, would be possible under time constraints, and could be combined with the subsequent optical design scheme—which requires that the dot density be both adjustable and controllable according to the luminance output from the optical design scheme. Chang et al.¹⁰⁻¹² have developed a random dot generation scheme that can accommodate the many needs of the optical design phase and have successfully integrated both procedures in dot pattern optimization. Random dot distribution possesses many advantages compared to regular dot distribution, such as both eliminating the moiré phenomenon^{13,14} arising from the interference of the light passing through the regular dot arrangement and making it easier to amend the dot distribution on the core plate (or cavity plate) by direct laser writing on the plate surface between the dots produced in a random dot distribu-

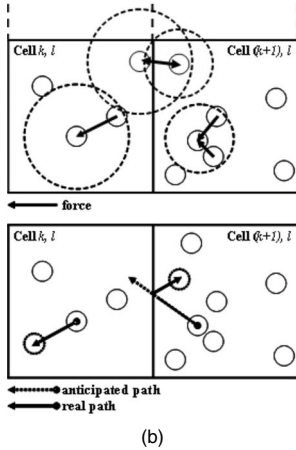
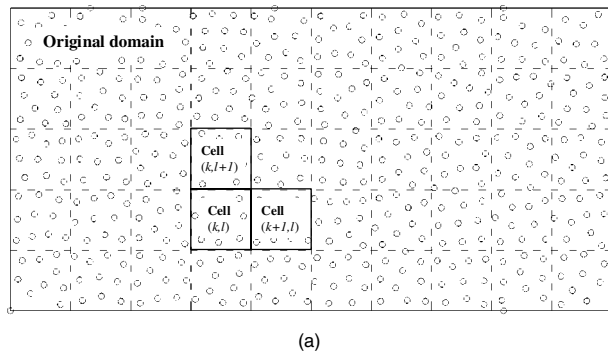


Fig. 1 (a) Schematic diagram of cell technique, the original domain being divided into a number of subdomains called cells. (b) The upper panel shows the variable r -cut technique, where the r -cut is large when the dot density in a cell is small and, conversely, the r -cut is small when the dot density in a cell is large. This is done by changing of the r -cut value in each cell to attain variable dot density. The force control parameter, c_{kl} , is averaged when the force field of the dot in cell kl is toward cell $(k+1)l$, as shown in upper part of the force field enclosed by the dashed circle. The lower panel shows the reflective boundary condition in each cell, where the dot will reflect back to its original cell if another dot is moving across the cell boundary.

tion.^{15–17} However, neither Chang et al.¹² nor Ide^{13,14} show the ability of the dot generation scheme to handle a thin light guide on an order of several million dots, which takes a significantly longer time to obtain uniform dot distribution after the molecular dynamics (MD) calculation of force regulation. This would limit the usage of the generation scheme to midsized backlights with a thin light guide, also called a thin backlight. Thus, the development of a more efficient generation scheme that can handle a large number of dots on the light guide is undoubtedly needed.

The objective of this study is to develop a dot generation scheme that can handle a typical backlight on the order of several millions dots for use in a midsized LED thin backlight. This scheme is based on the MD method and incorporates several new techniques—the periodic boundary condition and fixed-cell boundary condition—that geometrically reduce the MD calculation from that of the whole light guide domain to only a very small portion of the domain. This significantly reduces the computational effort and makes the generation scheme so efficient that the subsequent optical optimization of the dot pattern can be

done on a simple PC. After describing this present scheme, this paper takes as an application an example of a 14-in backlight to illustrate the validity of the scheme and to present the optical optimization of the dot distribution.

2 Mathematics Formulation

2.1 Motion Equation

The mass center of the microstructure can be considered as an atom, and its motion obeys Newton's second law, similar to the usual treatment in the MD method, such that

$$m \frac{d^2 \mathbf{r}_i}{dt^2} + c_d \frac{d\mathbf{r}_i}{dt} = \sum_j^n \mathbf{f}_{ij}(r_{ij}), \quad (1)$$

where $\mathbf{r}_i$ is the position of the i 'th atom, m is the atom mass, c_d is the damping term, $\mathbf{f}_{ij}$ is the force exerted on atom i by neighboring atom j , n is the total number of neighboring atoms around atom i , and $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$, with the final expression $\mathbf{f}_{ij}(r_{ij})$ (Ref. 10) being

$$\mathbf{f}_{ij}(r_{ij}) = \frac{\mathbf{r}_{ij}}{r_{ij}} \exp[-(r_{ij}c_{kl})], \quad (2)$$

where $r_{ij} = |\mathbf{r}_{ij}|$, c_{kl} is the force control parameter, and subscript k and l are the cell division row and column numbers, as shown in Fig. 1(a). Notice that in Fig. 1(a), the original domain is divided into several subdomains called cells. In these cells, every force parameter, c_{kl} , is the force control parameter, and subscripts k and l are the cell division in row number and in column number, as shown in Fig. 1(a). In Fig. 1(a), the original domain is divided into a number of smaller cells whose dot densities can be individually adjusted. As discussed in the following, the force control parameter, c_{kl} , is dependent on the dot density in each cell kl . In each cell kl , the force control parameter is given by:

$$c_{kl} = \frac{-\ln f_{re}}{r_{cut,kl}}, \quad (3)$$

where f_{re} is the residual force at the r -cut distance in each cell kl . It is noted that f_{re} tends toward zero when r_{ij} is larger than or equal to the r -cut distance, $r_{cut,kl}$. In general, a small value of a nonzero of f_{re} is used to consider the dot size in practice. During the force calculations, the neighboring atoms of each atom are identified using the Verlet algorithm,¹⁸ which reduces the n^2 search to an n search, and the force control parameter is determined according to their distances.

As described earlier, the proposed MD dot generation algorithm separates the domain of interest into a prescribed number of individual cells in order to enhance the flexibility of the dot density adjustment procedure. In one cell, kl , the dot density is defined as:

$$D_{kl} = \frac{A_{dot}}{A_{cell}} = \frac{m_{kl} \cdot \pi \cdot r^2}{A_{cell}}, \quad (4)$$

where m_{kl} is the total number of dots in cell kl , and r is the radius of the individual dots. In the current approach, each cell is considered to be rectangular, and it is assumed that the dot radius remains constant throughout the domain.

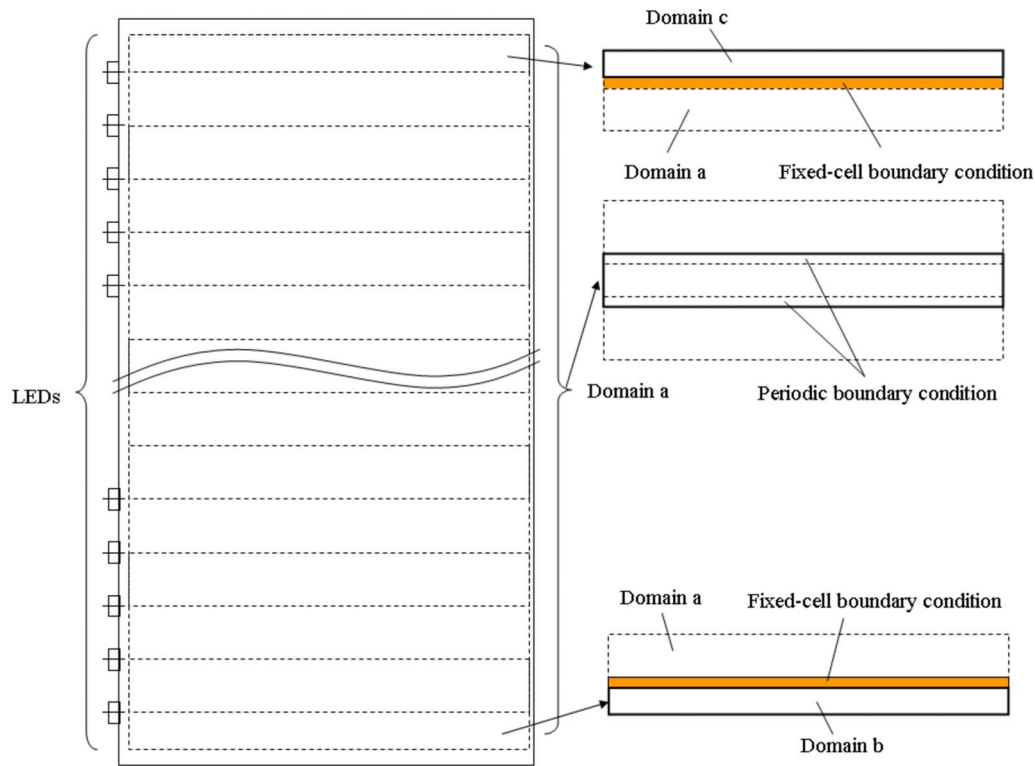


Fig. 2 Layout of a 14-in LED backlight and a schematic diagram showing the periodic boundary condition and fixed-cell boundary conditions that reduce the whole generation domain into three sub-domains, labeled *a*, *b*, and *c*. Domain *a* uses a periodic condition, and domains *b* and *c* use the fixed-cell boundary condition to generate the dot. Domain *a* contains many bands, while domain *b* and domain *c* contain only one band. A band is composed of numerous cells organized in layers longitudinally, each cell containing a specified number of dots, depending on distribution parameters.

2.2 Variable *r*-Cut Technique

In order to ensure that all of the dots in one cell can interact with all of their neighboring dots, the total area enclosed by the *r*-cut radius, $A_{r,kl}$, defined as the reactive area, should extend beyond the boundaries of the individual cell. In the limiting case, the smallest reactive area, $A_{r,min,kl}$, in cell *kl* is given by:

$$A_{r,min,kl} = \frac{A_{cell}}{m_{kl}}. \quad (5)$$

Equation (5) provides the minimum *r*-cut value. The actual *r*-cut value can then be obtained from:

$$r_{cut,kl} = a_m \cdot \left(\frac{A_{cell}}{\pi \cdot m_{kl}} \right)^{1/2}, \quad (6)$$

where a_m is a multiplier, and $m_{kl} = (D_{kl} \cdot A_{cell} / \pi r^2)$, from Eq. (4). Equation (6) indicates that the *r*-cut value is large when the dot density, which is equivalent to m_{kl} , is small. Conversely, it is small when the dot density is large, as seen in Fig. 1(b). For this reason, the present study refers to the task of specifying appropriate *r*-cut values for the variable *r*-cut technique.

Due to the fact that the *r*-cut value is adjusted according to the dot density of each cell, the force control parameter, c_{kl} , also varies with the change of *r*-cut value. In order to keep the dot distribution smooth across the cell boundary,

the control parameter of cell *kl* is averaged with that of the adjacent cell—for example, $k(l+1)$, when the region enclosed by $r_{cut,kl}$ exceeds the cell *kl* boundary into the cell $k(l+1)$, as seen in the upper panel of Fig. 1(b).

Although the *r*-cut value in a cell can be adjusted to different dot densities, during the force calculation to obtain uniform random distribution, it is difficult to prevent the dots from escaping from the cell into another cell. This leads the dot density in the cell after the force calculation to be different from the initial density. To prevent this dot number change, the reflective boundary condition is also imposed on each cell boundary to maintain the dot number as constant during the force calculation, as depicted in the lower panel of Fig. 1(b).

The base of the overall dot generation process is Eq. (1), subject to initial random data at a specific dot density distribution—the data having been provided from a random data generator, and that may include overlapping of dot data. The dots then repulse according to the force acting between them and reach their final equilibrium positions according to the simulated force calculation. This whole process of manipulating the force calculation until the dots reach their final equilibrium positions is hereafter simply referred to as force regulation.

2.3 Geometrical Condition

The previous Secs. 2.1 and 2.2 are general formulations for the random dot generation and for obtaining the uniform

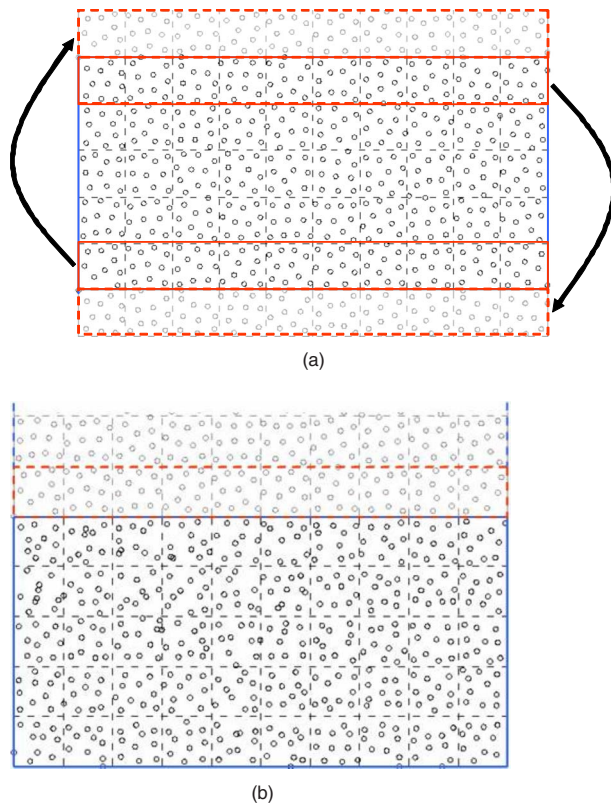


Fig. 3 (a) Schematic diagram of the periodic boundary condition. The two areas enclosed by the red line represent the topmost and bottommost cells in one band. The gray dot areas are the mapping areas related to the topmost and bottommost cells. (b) The fixed-cell boundary condition is represented by the well-arranged gray dots in the upper part marked with a dotted red line; they remain unchanged at their positions. The dots in the lower part are expected to obtain the uniform random dot distribution after force regulation. (Color online only.)

random dot distribution after the force regulation, done without the benefit of reducing the number of necessary domain calculations that our dot generation scheme provides by using the periodic boundary and fixed-cell boundary conditions. Employing these geometrical conditions increases the ability to handle the distribution of a large number of dots for use on the base of the light guide.

Figure 2 shows the layout of a 14-in light guide, which has 40 LED light sources along its left edge. The geometrical conditions depicted in the right panels of Fig. 2 are used to reduce the number of dots employed in the dot generation scheme. The first is the periodic boundary condition, labeled as *a*, which generates the dots in the domains extending from each LED but does not affect the last domain on either end of the light guide. Here, we make an assumption in applying the periodic condition such that the discrepancy of each LED light source is assumed to be negligible. In fact, in the optical design phase, each LED light source is set using identical specifications. The second geometrical condition is that of the fixed-cell boundary condition, which generates a continuous-change dot pattern distribution in the uppermost and lowermost domains, labeled as *c* and *b*, respectively. The use of these two conditions is the most efficient way to reduce the large number of dots

used in the dot generation scheme. The reason for the use of the periodic condition rather than another geometrical condition, such as the symmetry condition, is that the dot pattern needs to be repeatable such that there is no distinguishable border between adjacent bands, which causes visual defects of dark stripes on the backlight. The domains at both ends, labeled as *b* and *c*, are not suitable for the periodic condition because there is no LED light source in those areas adjacent to domain *a*. To avoid a discontinuous dot pattern across the topmost domain boundary, the upper part of domain *a* (which borders domain *c*), marked as the gray region, must utilize a fixed-cell boundary condition, which can pass the acting force onto the dots of the lower part of domain *c* (which borders domain *a*). The same condition is true for the lower part of domain *a*, as it contacts the upper part of domain *b* with a fixed-cell boundary condition.

In the following sections, the details of these two boundary conditions are provided.

2.3.1 Periodic boundary condition

The schematic diagram of the periodic boundary condition for domain *a* is shown in Fig. 3(a). Part of the benefit of using the periodic boundary condition is that calculations need be made for only one band, which can then be repeated throughout domain *a*. In order for continuity of these repeated bands, the single band is calculated so that the cells of the bottom of the band are mapped as if they bordered the topmost cells of the band, and vice versa. The single band can then be duplicated as necessary with total continuity. In addition, should it be necessary (although in this light guide, it is not) the leftmost cells can be similarly mapped as if they bordered the rightmost cells, to make the geometry extendable along these two directions. Using these parameters, the dot pattern can become truly periodic and extendable in all directions.

2.3.2 Fixed-cell boundary condition

The schematic diagram of the fixed-cell boundary condition is depicted in Fig. 3(b). This condition requires a two-step process. The dots in the cells at the outer edge of domain *a* are first suitably arranged by force regulation. Next, they are selected and fixed at the outer edge of the domain and are used for the force regulation for the domain adjacent to it—domain *c* for the top of domain *a*, and domain *b* for the bottom. Although the dot positions are fixed during the force regulation, the force still acts on the other moveable, unfixed, dots in the adjacent domain. The use of this fixed-cell boundary condition allows for dot pattern generation in a step-by-step manner, first doing the force regulation for one domain and fixing the fixed-cell boundary condition for the next adjacent domain, and then doing the force regulation again to obtain the new dot arrangement. From the theoretical MD viewpoint previously introduced, it is not necessary to select the whole domain as the fixed-cell boundary condition. A thickness of only one adjacent cell is enough to act as the boundary condition because the *r*-cut is restricted in one cell (see Sec. 2 for explanation)—that is, the interaction force distance between dots is not longer than one cell.

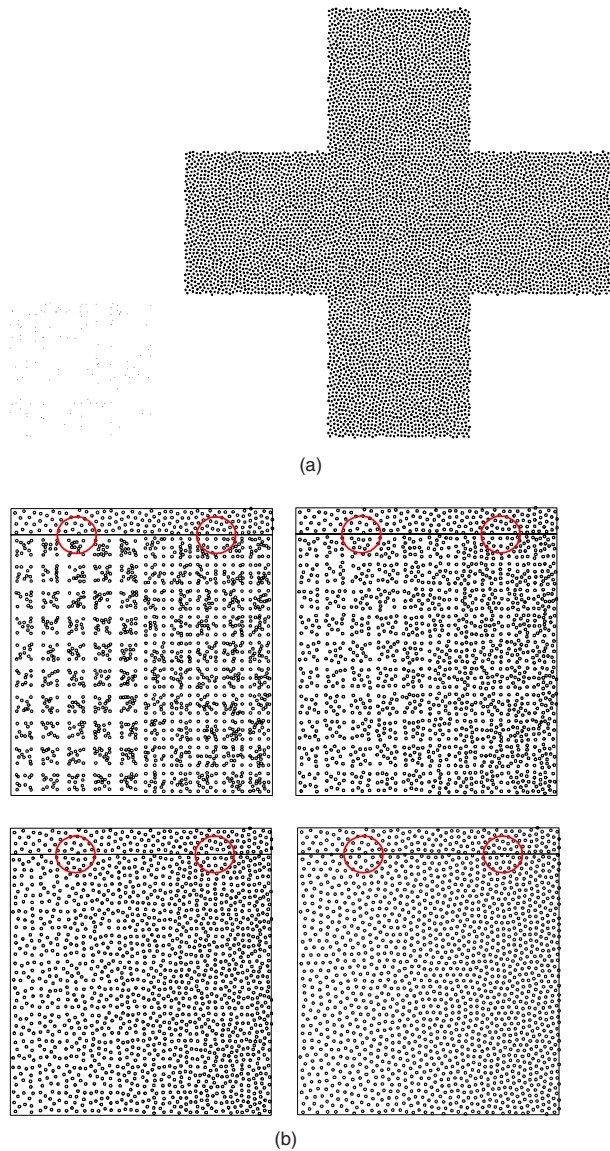


Fig. 4 (a) Dot pattern with the periodic boundary condition and its assembly extending in the up, down, left, and right directions. (b) Sequences of dot pattern generation by the fixed-cell boundary condition.

3 Results and Discussion

Before explaining a practical case of a 14-in backlight, two illustrations are presented to show the validity of the use of the periodic boundary condition and fixed-cell boundary condition to generate dot distribution. Figure 4(a) shows the dot distribution generated by using the periodic boundary condition, where the upper panel shows a single hypothetical domain of the dot distribution, and the lower panel shows the assembly of four such single domains, extending to the right and left, as well as up and down. Note that the dot distribution is continuous without distinguishable boundaries. The use of the periodic boundary condition to generate dot distribution provides a great advantage in that a smaller domain can be used to reproduce the dot distri-

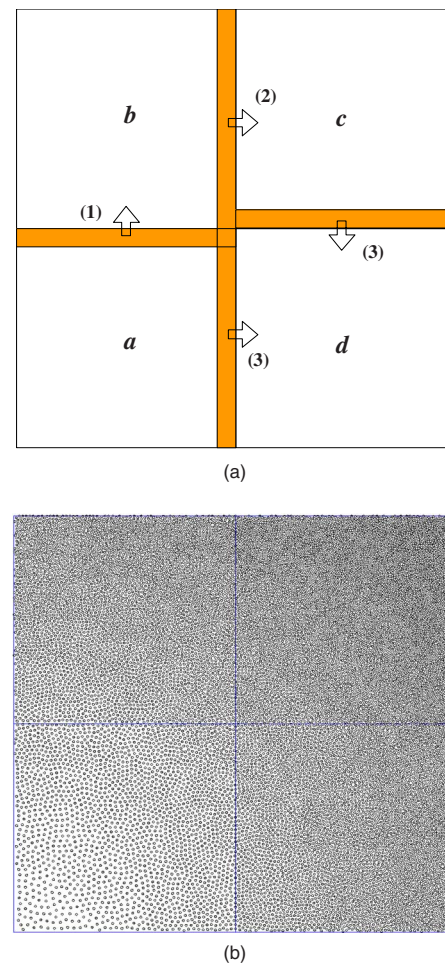


Fig. 5 Clockwise pattern structure generated in a step-by-step manner by using the fixed-cell boundary condition. (a) Schematic diagram of successive building blocks and the related fixed-cell boundary conditions. (b) The final dot distribution (domain $a=2,415$ dots; domain $b=3,935$ dots; domain $c=5,435$ dots; and domain $d=4,790$ dots).

bution of a large area. Not only is this more efficient, but it is also especially useful if the dot distribution of a constant density needs to be generated.

Figure 4(b) shows a snapshot sequence of the dot distribution at the beginning, intermediate, and final stages during the force regulation. The horizontal line represents the boundary between adjacent domains. In the upper part of the diagram (representing the lower edge of the upper adjacent domain), the dot distribution remains in fixed positions, with the fixed-cell boundary condition imposed on the boundary cell. The dots in the lower part of the diagram (the lower domain) are expected to obtain uniform dot distribution by MD force regulation and display continuous dot distribution across the domain boundary. The snapshot sequence shows that the dot distribution in the lower domain becomes uniformly distributed by the end of force regulation. A close inspection of both domains close to the boundary throughout the sequence is shown by the red circles. In the right circle, the dots in the fixed-cell boundary are denser, with a vacancy along the boundary. The dots of the lower domain move to fill in the vacancy, the end result being dots clustered more densely than in the left

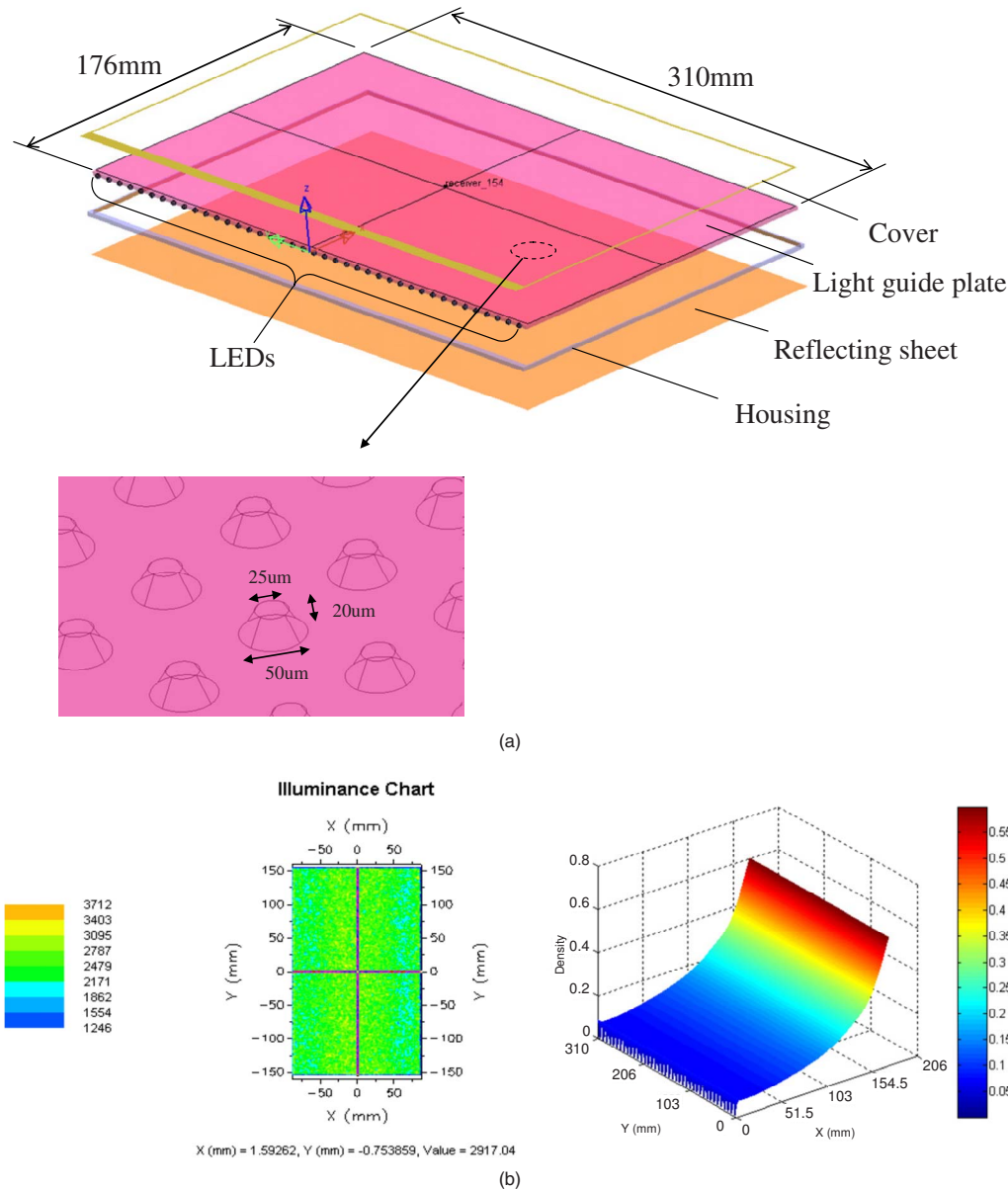


Fig. 6 (a) Schematic diagram of the optical model for the light guide module. (b) Illuminance distribution and the related dot density distribution.

circle. In the left circle, a dot—rather than a vacancy—exists along the boundary. The dots of the lower domain are repulsed, the end result being dots clustered less densely than in the right circle. Although the dots remained fixed, the forces still act not only within the fixed-cell domain but also on the region outside those fixed cells. In addition, the boundary between the dot distribution domains is difficult to differentiate.

Figure 5 shows a dot distribution, the density of which increases when moving clockwise starting from the lower-left corner. The dot distribution is constructed in a step-by-step manner, where the dot distribution is built in one domain at a time, as shown in Fig. 5(a), where *a*, *b*, *c*, and *d* are one-quarter of the total area. The procedure begins from domain *a* first, where the dot distribution is constructed by the force regulation process. Next, the area bordering do-

main *b*, marked in orange, is recorded and set as the fixed-cell boundary condition for use in building the next domain. This process is repeated, successively constructing the whole area, with each 'orange area' representing those areas that become fixed for the construction of the subsequent domain. Note that two fixed-cell boundary condition areas are needed for the last domain *d*. The final result, as shown in Fig. 5(b), shows a very smooth dot distribution and no easily distinguishable boundary between two domains. In this example, we have illustrated that the dot distribution of a large domain can be constructed by decomposing the whole domain into several subdomains by employing the fixed-cell boundary condition. The computational time consumed was also reduced in this example, with the average time used for a quarter of the whole do-

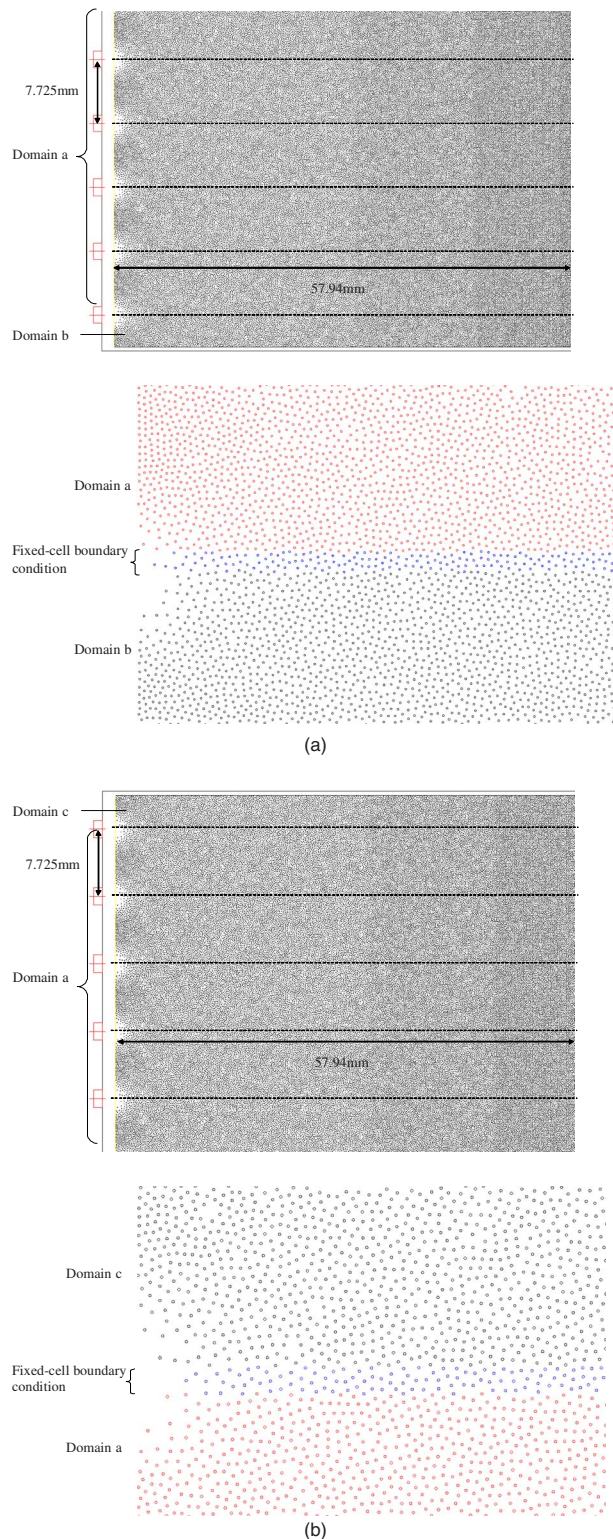


Fig. 7 (a) Upper panel: Dot distribution for the lower part of light guide. Lower panel: Enlarged view of the dot distribution for the upper panel across domains *a* and *b*. (b) Upper panel: Dot distribution for the upper part of the light guide. Lower panel: Enlarged view of the dot distribution for the upper panel across domains *a* and *c*. In both (a) and (b) enlarged views, the light blue dots represent the fixed-cell boundary condition. (Color online only.)

main being about 23 min, while previous methods that computed the whole domain required about 131 min.^{10–12}

Returning to the dot generation for use in a 14-in backlight application (shown in Fig. 2), we find that the subsequent optical optimization, as well as the remove-from or add-on techniques of dot distribution during MD force regulation process, can be derived mostly from our former research.¹² In a previous study¹¹ for the optical optimization, we proposed the simple proportional rule that the output illuminance is proportional to the dot density of the cell and that the dot density of each cell can be updated depending on the illuminance output of the related cell area. Here, only slight modifications are necessary to update the dot density for the repeated domain *a* by using the optical design analysis average illuminance results for the related domains. The optical optimization can be automatically iterated by combining Visual Basic (VB), the dot generation program proposed in this study, and LightTools software to reach the uniformity condition. Figure 6(a) shows the schematic diagram of an optical model of the backlight module that contains 40 LEDs, each of which has an intensity of 1300 mcd and an angle of half intensity of 60 deg. The dot structure is a truncated cone, which is constituted of a conical structure with a flat, truncated top surface, shown in the inset of Fig. 6(a). The optical properties of these surfaces are assumed to obey Fresnel's reflection and transmission equations. Figure 6(b) shows the final illuminance and the dot density distribution when the uniformity condition is reached. The original number of dots at the beginning of the first iteration is 4,695,480. The final total dot number is 3,641,933, where domains *a*, *b*, and *c* have 89,763, 73,372, and 67,804 dots, respectively. The process required a total of 34 iterations, and the computational time for each iteration averaged about 1.5 h. Thus, total computational time consumption was about 51 h. For comparison, the method using the whole areas as a single domain, as in the previous method described by Chang et al.^{10–12} for MD force regulation, required 70 h of computation to reach uniform random distribution over one iteration when starting from the same total dot number. Note that this computation has not yet met the uniformity requirement. Clearly, the employment of the geometrical conditions offered in this paper can significantly shorten the computational time to reach a uniform random dot distribution and make dot optimization possible by reaching the uniformity requirement.

Last, Fig. 7 shows an enlarged view of the dot distribution from above in order to examine the continuity of the dot distribution across domains *a* and *b* [Fig. 7(a)] and domains *a* and *c* [Fig. 7(b)]. In Figs. 7(a) and 7(b), the upper panels show the parts of the dot distribution at the lower and upper edges of the light guide, respectively. The lower panels in Figs. 7(a) and 7(b) show an enlarged view of the upper panels. In the enlarged views, we can clearly examine the continuity of the dot distribution across domains *a* and *b* and domains *a* and *c*. That the dot distribution is continuous across the boundaries between domains validates the present approach.

4 Conclusions

This paper proposes a dot pattern generation scheme based on the MD method by incorporating the periodic boundary condition and fixed-cell boundary condition to deal with the

optical optimization of the dot pattern of an LED thin light guide with a large number of dots. The periodic boundary condition utilizes a dot pattern with repeatable characteristics such that only one pattern is necessary to represent the entire area. The fixed-cell boundary condition can extend the continuity of the dot distribution by imposing this condition prior to the force regulation of an adjacent domain in a step-by-step manner. By taking advantage of these two geometrical conditions, the generation scheme can significantly reduce computational efforts and separate the whole domain calculation into only three individual subdomain calculations to reach a uniform random distribution for the LED thin backlight. This allows the ability for dot pattern generation, as well as dot pattern optimization, to extend to the order of several million dots in order to meet the design requirement of the LED thin backlight. The practical example of a 14-in backlight also shows the validity of the present proposed scheme.

Acknowledgments

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