# Analysis of Ion Implantation Profiles for Accurate Process/Device Simulation: Ion Implantation Profile Database Based on Tail Function

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In the design of very-large-scale integrated circuit (VLSI) devices, accurate prediction of the doping profiles resulting from ion implantation, a standard method for doping impurities in VLSI processes, is essential. This is done by obtaining analytical expressions for the secondary ion mass spectrometry (SIMS) data of ion implantation profiles, and these analytical formulas are used to compile an ion implantation profile database. The profiles of arbitrary implantation conditions can be generated using interpolated parameter values. The functions used to express these ion implantation profiles include Gaussian, joined half Gaussian, Pearson, and dual Pearson functions. In addition to these, my coworkers and I have proposed a new tail function. This tail function has fewer parameters than the dual Pearson function, which is currently the standard function used in general-purpose simulators, and it is better able to specify an arbitrary profile using a unique set of parameters. We used this function to construct an ion implantation database comprising approximately 1000 smaller databases. By linking this database with a single additional parameter, we were also able to predict the amorphous layer thickness under a wide range of implantation conditions.

## 1. Introduction

Ion implantation is a standard doping technique for semiconductor materials, and accurate predictions of the resulting ion implantation profiles are essential for process development. For this purpose, efforts are being made to construct a database. The ion implantation conditions used in very-large-scale integrated circuit (VLSI) processes include the species, energy, and dose of the implanted ions, the implantation angle, and the substrate material, so the database is very large. As the first step in constructing a database, the implantation profiles of ions implanted under various different conditions are evaluated by secondary ion mass spectrometry (SIMS). Functions that reproduce these profiles are prepared, and their parameter values are optimized to fit the SIMS data. The functions' parameter table is essentially what constitutes the database. Profiles obtained under arbitrary ion implantation conditions can be predicted by interpolating these parameter values. Accordingly, the quality of the database depends largely on the functions incorporated within it. It goes without saying that these functions should be capable of accurately expressing all the experimental data without exception. They should also be implemented using unique parameter sets for the reasons described below.

When one database is combined with another, any inconsistencies between their parameter values will make it necessary to either use just one database or to extract the parameter values again from scratch in order to achieve useful database integration. Unique correspondence between parameter sets and implantation profiles is therefore essential when forming a large database by combining various smaller ones.

When ions are implanted into a crystalline substrate, the crystal structure may be completely destroyed under some conditions to form a continuous amorphous layer. Ion implantation channeling phenomena behave differently depending on whether or not this amorphous layer is present. Research is even being carried out into techniques where an amorphous layer is deliberately formed to prevent the impurities from diffusing, thereby achieving higher activation states.<sup>1)-5)</sup> It is therefore important to understand the extent to which amorphous layers are formed under various different ion implantation conditions.

In this paper, I introduce the functions that have been proposed to date for representing ion implantation profiles and discuss their benefits and drawbacks. I then introduce a tail function that my coworkers and I proposed to resolve the problems with these functions. I also introduce a model for predicting the thicknesses of amorphous layers formed by ion implantation. The database based on these models covers almost the entire range of ion implantation conditions used in modern VLSI processes.

#### 2. Moments of profile

When a profile N(x) is obtained, the basic information about it can be expressed in terms of moments as follows:

• First-order moment The first-order moment  $R_p$  is defined as

$$R_p = \frac{\int_0^\infty x N(x) \, dx}{\int_0^\infty N(x) \, dx} \,. \tag{1}$$

This corresponds to the average depth reached by the ions, as shown in **Figure 1**. The moment  $\mu_i$  for an arbitrary index *i* is calculated from the following formula:

$$\mu_{i} = \frac{\int_{0}^{\infty} (x - R_{p})^{i} N(x) dx}{\int_{0}^{\infty} N(x) dx} .$$
<sup>(2)</sup>

Second-order moment

The formula for  $\Delta R_p$  associated with the second-order moment is

$$\Delta R_p = \sqrt{\mu_2} \quad . \tag{3}$$

As shown in Figure 1, this formula corresponds to the standard deviation, which expresses the degree of spreading in the  $R_p$ profile. The concentration at a depth of  $R_p+\Delta R_p$ is approximately half the peak concentration. Parameters  $\gamma$  and  $\beta$  in Figure 1 are given by Equations (4) and (5).

#### Third-order moment

The parameter associated with the thirdorder moment is called skewness and is given by

$$\gamma = \frac{\mu_3}{\Delta R_p^3} \,. \tag{4}$$

It is negative if the distribution is skewed in front of  $R_p$ , positive if it is skewed behind  $R_p$ , and zero if the distribution is symmetrical. The dependence of the distribution on  $\gamma$  is shown



Figure 1 Description of profile parameters  $R_{\rho}$  and  $\Delta R_{\rho}$ .

in **Figure 2**. A larger value of  $\gamma$  results in a more asymmetric distribution. In Figure 2,  $\gamma$  takes positive values, but the distributions for negative values can be obtained by reflecting the distributions about an axis positioned at  $R_p$ .

Fourth-order moment

The parameter associated with the fourthorder moment is called kurtosis and is given by

$$\beta = \frac{\mu_4}{\Delta R_p^4} \,. \tag{5}$$

It describes how sharp the profile is in the vicinity of the peak. For the Gaussian distribution discussed in the next section,  $\beta=3$ . As shown in **Figure 3**, if  $\beta>3$ , the profile has a sharper peak and a broader base, while if  $\beta<3$ , the profile has a gentler peak and drops off more sharply at the base.

These moment parameters provide basic information about the distribution. The accuracy of the functions used to express distribution profiles depends on which parts of this information are used.

Although distributions depend on moments beyond the fourth order, as shown by Equation (2), we limit our treatment to moments up to the fourth order for the functions introduced in the next section. However, we should point out



Figure 2 Effect of  $\gamma$  on profile shape.

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that since higher-order moments incorporate information about errors at lower concentrations in the experimental data, using higher-order moments for practical problems will not necessarily simply lead to greater precision. One function that can consider higher-order moments is the Edgeworth series,<sup>6)</sup> but unless it is treated using higher-order moments, the resulting distributions can oscillate in ways that are impossible in practice. As a result, they are seldom used today.

## 3. Dual Pearson standard function

Here, I give a simple introduction to functions that express ion implantation profiles by using the moment parameters shown in the previous section.

The simplest formula for expressing an ion implantation profile is a Gaussian distribution. A Gaussian distribution is expressed in terms of first- and second-order moment parameters  $R_p$  and  $\Delta R_p$  as

$$N(x) = N_m \exp\left[-\frac{(x-R_p)^2}{2\Delta R_p^2}\right],$$
(6)

where  $N_m$  is the peak concentration, which is



Figure 3 Effect of  $\beta$  on profile shape.

expressed in terms of the implantation dose  $\Phi$  as

$$N_m = \frac{\Phi}{\sqrt{2\pi}\Delta R_p} \ . \tag{7}$$

These formulas can be used to directly obtain an idea of the distribution. This function specifies that the distribution is symmetrical about  $R_p$  ( $\gamma$ =0). However, real ion implantation profiles are often asymmetrical. To express the asymmetry of distributions, Gibbons et al. proposed a joined half Gaussian profile consisting of two Gaussian profiles with different values of  $\Delta R_p$  joined at the peak position.<sup>7)</sup> This profile is given by

$$N(x) = \begin{cases} N_m \exp\left[-\frac{\left(x - R_{pm}\right)^2}{2\Delta R_{pf}^2}\right] & \text{for } x \le R_{pm} \\ \\ N_m \exp\left[-\frac{\left(x - R_{pm}\right)^2}{2\Delta R_{pb}^2}\right] & \text{for } x > R_{pm} , \end{cases}$$
(8)

where  $R_{pm}$  is the depth of the peak concentration  $N_m$ ,  $\Delta R_{pf}$  is the standard deviation of the Gaussian profile between  $R_{pm}$  and the surface, and  $\Delta R_{pb}$  is the standard deviation of the Gaussian profile below  $R_{pm}$ . The peak concentration  $N_m$  is given by

$$N_m = \sqrt{\frac{2}{\pi}} \frac{\Phi}{\Delta R_{pf} + \Delta R_{pb}} \,. \tag{9}$$

This can be used to express the profile's asymmetry.

The profile of B ions implanted into an amorphous Si substrate at 80 keV is shown in **Figure 4**. Here, the SIMS profile corresponds to SIMS analysis results. A Gaussian distribution cannot express this asymmetric profile. And although a joined half Gaussian can provide a good representation of the peak depth and the neighborhood of the peak, it cannot represent profiles that decrease exponentially towards the surface. A strong limitation of joined half Gaussian profiles is that the values of exponential terms vary with the square of the distance. This makes it impossible for this function to express the exponential functions that are seen in the low-concentration region near the surface. Accordingly, these functions are not used for database construction.

Although Gaussian and joined half Gaussian functions are not used for database construction because of their inability to express all profiles, they can represent many different profile types. They are simpler and easier to work with than Pearson functions (described below), so they are widely used in data analysis applications.

As the equations clearly show, the only parameters that the Gaussian and joined half Gaussian functions make explicit use of are the  $R_p$  and  $\Delta R_p$  moment parameters (i.e., those are the only parameters that actually appear in the formulas). The joined half Gaussian function also makes implicit use of  $\gamma$  (i.e., it affects the function without actually appearing in the formula). A Pearson profile uses moments up to the fourth order<sup>8),9)</sup> and is derived from the following differential equation.



Figure 4 Representations of implantation profiles with Gaussian, joined half Gaussian, and Pearson functions.

$$\frac{dh(s)}{ds} = \frac{(s-a)h(s)}{b_0 + b_1 s + b_2 s^2},$$
(10)

where  $s = x-R_p$ , and the coefficients *a*,  $b_0$ ,  $b_1$ , and  $b_2$  are associated with the moments shown in the previous section. The Pearson function forms function classes I–VII in **Figure 5**. Of these functions, Pearson IV is the most commonly used one: it is given by

$$h(s) = K \left| b_0 + b_1 s + b_2 s^2 \right|^{\frac{1}{2b_2}} \times \exp\left[ -\left(\frac{b_1}{2b_2} + a\right) \frac{2}{\sqrt{4b_2 b_0 - b_1^2}} \tan^{-1} \left(\frac{2b_2 s + b_1}{\sqrt{4b_2 b_0 - b_1^2}}\right) \right].$$
(11)

The coefficients a,  $b_0$ ,  $b_1$ , and  $b_2$  in this case are associated with the moments, as shown below.

$$b_{0} = \frac{4\beta - 3\gamma^{2}}{10\beta - 12\gamma^{2} - 18} \Delta R_{p}^{2}$$
(12)

$$b_1 = -\frac{\beta + 3}{10\beta - 12\gamma^2 - 18}\gamma \Delta R_p \tag{13}$$

$$b_2 = -\frac{2\beta - 3\gamma^2 - 6}{10\beta - 12\gamma^2 - 18} \tag{14}$$



Figure 5 Regions occupied by Pearson function types in  $\gamma^2 - \beta$  plane.

$$a = b_1 \tag{15}$$

Coefficient K is determined by adjusting the dose to the desired value. To obtain a class IV Pearson profile,  $\beta$  must satisfy

$$\beta > \frac{3(13\gamma^2 + 16) + 6(\gamma^2 + 4)^{\frac{3}{2}}}{32 - \gamma^2} .$$
 (16)

However, an evaluation of moments in SIMS profiles shows that there are many cases where this condition is not met. In such cases,  $\beta$  is often taken to be the limiting value of Equation (16).

The reason Pearson IV profiles are especially popular among the class of Pearson functions is that, unlike the others, they are defined for all depths and are easy to work with. Although precise results can be obtained by selecting a compatible Pearson profile, here we use Pearson profiles without limitation to class IV (the formulas for classes I–VII can be found in Reference [9]).

Unlike elementary functions such as the Gaussian and joined half Gaussian, the profiles that result from Pearson functions are not easy to visualize. However, if the moments of the distribution are evaluated up to the fourth order, Equations (12)-(15) can be used to perform the calculations easily. The same applies to the other Pearson functions. As shown in Figure 4, Pearson functions can represent profiles that cannot be represented with Gaussian or joined half Gaussian functions and are used as basic functions for ion implantation profile representation. However, Pearson profiles do not have functions that can ultimately be used to construct a database for the following reason.

When ions are implanted into crystalline Si, a higher implantation dose causes more damage to accumulate in the crystalline matrix. At low doses, the defect regions grow in proportion to the dose, but beyond a certain dose they start to coalesce and finally result in a saturated state where a continuous amorphous layer is formed. Consequently, the substrate environments through which the ions travel are different between low-dose and high-dose implantation conditions. In other words, the number of channeling ions decreases as the dose increases, so the resulting implantation profile does not bear a linear relationship to the dose, and the parameters are dose-dependent even at the same implantation energy.

To avoid this problem, Tasch has proposed a dual Pearson profile whereby a single profile is divided into an amorphous part  $h_a$  and a channeling part  $h_c$ , and separate Pearson profiles are applied to each part.<sup>10),11)</sup> In other words, the distribution for a certain acceleration energy is expressed by

$$N(x) = (\Phi - \Phi_{chan}) h_a(x) + \Phi_{chan} h_c(x), \qquad (17)$$

where  $\Phi$  is the dose and  $\Phi_{chan}$  is the channeling dose, which is the dose of channeling constituents. A dual Pearson ion implantation profile is represented by the following nine parameters:

- $R_p, \Delta R_p, \gamma, \beta$  (moments associated with  $h_a$ )
- $R_{p2}, \Delta R_{p2}, \gamma_2, \beta_2$  (moments associated with  $h_c$ )
- $\Phi_{chan}$ . In a dual Pearson profile, the dose



Figure 6

Use of dual Pearson function to represent dose dependence of ion implantation profiles.

dependence of the overall profile can be accurately represented by varying the dose ratio of the two profile parts, as shown in **Figure 6**. Dual Pearson profiles are currently the standard functions incorporated into general-purpose simulators, and they can accurately represent the ion implantation profiles obtained under a wide range of conditions without exceptions.

## 4. Proposed tail function

The dual Pearson function can model ion implantation profiles closely, but when we attempt to fit real data to it so that it can be used to construct a database, it runs into problems with regard to the second requirement, namely, the issue of uniqueness.

As shown in **Figure 7**, it is possible to match the same profile even when various different values of  $R_{p2}$  are chosen. The values of the other corresponding parameters are also completely different, as shown in the figure. In other words, various different parameter sets can simultaneously represent the same profile with high precision. This makes the setting of  $h_c$  somewhat arbitrary and causes problems due to the lack of uniqueness in the parameters needed to represent a profile.

To alleviate this uniqueness issue, we proposed a tail function.<sup>12)-15)</sup> With this function, a single implantation profile is still represented using two profiles  $n_a$  and  $n_c$  for the amorphous and channeling parts, respectively.

$$N(x) = (\Phi - \Phi_{chan}) n_a(x) + \Phi_{chan} n_c(x)$$
(18)

Here, profile  $n_a$  is represented by a Pearson profile  $h_{ma}$ , i.e.,

$$n_a(\mathbf{x}) = h_{ma}(\mathbf{x}),\tag{19}$$

while  $n_c(x)$  uses a Pearson profile for the region near the peak and the combination of a Pearson profile and a tail function  $h_{Tc}$  for the tail region, i.e.,



Figure 7 Representation of ion implantation profile with dual Pearson profiles having different moment parameters.

$$n_{c}(\mathbf{x}) = \begin{cases} h_{mc}(\mathbf{x}) & \text{for } \mathbf{x} \le \mathbf{x}_{T} \\ \kappa \left[ h_{mc}(\mathbf{x}) + h_{Tc}(\mathbf{x}) \right] & \text{for } \mathbf{x} > \mathbf{x}_{T}. \end{cases}$$
(20)

Functions  $h_{ma}$  and  $h_{mc}$  have the same moment. The tail function is given by

$$h_{T_c}(x) = h_{mc}(x_p) \exp\left[-(\ln \eta) \left(\frac{x - x_p}{L}\right)^a\right].$$
 (21)

Here,

$$x_T = R_p + \Delta R_p \tag{22}$$

and  $x_p$  is the position of the peak concentration.  $\kappa$  is determined from the continuity condition at  $x = x_T$  according to

$$h_{mc}(x_{T}) = \kappa \Big[ h_{mc}(x_{T}) + h_{Tc}(x_{T}) \Big].$$
(23)

Here,  $\eta$  is an arbitrary parameter that was set to a fixed value of 1000 in this study. It signifies that the concentration at a place separated from  $x_p$  in Equation (21) by a distance of L is one thousandth of the peak concentration. The shape of the tail is expressed by parameter a, which is 1 for an exponential distribution and



Figure 8 Tail function representation of ion implantation profile.

2 for a Gaussian distribution. In other words, parameters L and a are directly connected to the profile shape and do not suffer from the ambiguity that occurs with the parameters  $R_{p2}$ ,  $\Delta R_{p2}$ ,  $\gamma_2$ , and  $\beta_2$  of dual Pearson profiles. The tail function has 7 parameters,  $R_p$ ,  $\Delta R_p$ ,  $\gamma$ ,  $\beta$ , L, a, and  $\Phi_{chan}$ , which is two fewer than the dual Pearson function. With this function, a single profile can be represented as shown in **Figure 8**. We checked that this function can accurately represent all profiles that can be represented

Table 1 lons, substrates, and ions' energy-ranges covered by database.

lon	Substrate	Energy range (keV)
В	c-Si	0.5–2000
Р	c-Si	1–2000
As	c-Si	1–300
Sb	c-Si	1–300
In	c-Si	1–300
BF <sub>2</sub>	c-Si	0.5–60
Ge	c-Si	5–160
Si	c-Si	20–160
С	c-Si	5–300
Ν	c-Si	5–300
F	c-Si	5–300
Ar	c-Si	10–160
В	a-Si	0.5–2000
Р	a-Si	1–160
As	a-Si	1–160
Sb	a-Si	1–300
BF <sub>2</sub>	a-Si	0.5–60
В	poly-Si	2.5–40
Р	poly-Si	2.5–80
As	poly-Si	2.5–80
В	SiO <sub>2</sub>	0.2–160
Р	SiO <sub>2</sub>	1–160
As	SiO <sub>2</sub>	1–160
В	HfO <sub>2</sub>	3–20
Р	HfO <sub>2</sub>	5–80
As	HfO <sub>2</sub>	5–80
В	Ge	3–80
Р	Ge	5–80
As	Ge	10–80

c-Si: crystal Si a-Si: amorphous Si poly-Si: polycrystal Si

with a dual Pearson function. In all cases, we were able to reproduce the experimental data to a high level of accuracy, allowing us to construct a database covering all the conditions in **Table 1**.

### 5. Amorphous layer thickness

When heavy ions are implanted into a crystalline substrate, defect regions are formed along the paths of the implanted ions. As the dose increases, these defect regions overlap and



20 nm

#### Figure 9

Cross-sectional transmission electron microscopy image of amorphous layer formed by Ge ion implantation.



Figure 10

Fabrication of shallow junction by Ge ion implantation to form amorphous layer.

ultimately form a continuous amorphous layer. A cross-sectional transmission electron microscopy image of a Si substrate implanted with 10-keV Ge ions at a dose of  $1 \times 10^{15}$  cm<sup>-2</sup> is shown in **Figure 9**. For these conditions, it is possible to see a clear interface between the amorphous and crystalline regions (a/c interface), and the amorphous layer thickness  $d_a$  is approximately 30 nm.

Distributions of B ions implanted into substrates with and without an amorphous layer formed by Ge ion implantation are shown in **Figure 10**. The depth at which the concentration reached  $10^{18}$  cm<sup>-3</sup> differed by a factor of approximately 2 between the two cases. Thus, if an amorphous layer is formed and ion implantation is used to add impurities into this amorphous layer, a shallow junction is obtained with no channeling tail.

The variation in sheet resistance with annealing time at 600°C in substrates with and without an amorphous layer formed by Ge ion implantation is shown in **Figure 11**.<sup>5)</sup> These results show that by forming an amorphous layer and allowing it to recrystallize at a low temperature, it is possible to obtain low resistivity over a wide time range. It has been confirmed



Figure 11

Variation in sheet resistance of B ion implantation layer during annealing in substrates with and without amorphous layer formed by Ge implantation.

that this phenomenon is not intrinsic to Ge and can also be observed in amorphous layers formed by other impurities where recrystallization is allowed to take place at temperatures that produce little redistribution of impurities.<sup>1)-5)</sup>

Accordingly, in order to predict implantation profiles and activation behavior, it is essential to ascertain the approximate depth  $d_a$  of amorphous layers formed by ion implantation.

This defect formation mode was studied by Hobler et al. using Monte Carlo simulation.<sup>16)</sup> On the basis of an empirical treatment of this phenomenon, we have proposed simple parameters that influence the amorphous layer and have thereby made it possible to predict the amorphous layer thickness under a wide range of ion implantation conditions.<sup>17)–19)</sup> This model is introduced below.

The implanted ions travel through the Si lattice while interacting with it to form defects and finally come to rest in the Si. As shown schematically in **Figure 12**, we can imagine that a single ion forms a cylindrical defect region of length  $L_d$  and area  $\sigma$ . As the number of implanted ions increases the number of defect regions increases. The number of defect regions can increase until they cover the whole area cross section at a certain depth. At this point we can say that the implanted ions have turned the



Figure 12 Schematic illustration of defect formation.

Si into amorphous Si. The total area of defects regions per unit area  $S_{amo}(x)$  formed by the ions at depth x is given by

$$S_{amo}(x) = \sigma \int_{x}^{x+L_d} N(x) \, dx$$
  

$$\approx \sigma \int_{x}^{\infty} N(x) \, dx \,, \qquad (24)$$

where  $x+L_d$  is approximated by infinity in the integration range. In other words, as an approximation, we consider that the concentration of ions drops abruptly after they have traveled a distance  $L_d$  from x. When this area ratio  $S_{amo}$ reaches 1, an amorphous layer starts to form and the integral is assumed to take the value  $\Phi_{a/c}$ (called the through dose), i.e.,

$$1 = \sigma \int_{d_a}^{\infty} N(x) \, dx$$
$$= \sigma \, \Phi_{q'_a}. \tag{25}$$

Since  $d_a$  is known empirically, we can easily evaluate  $\Phi_{a/c}$  by integrating the distribution of actual experimental data beyond depth  $d_a$ , as shown in **Figure 13**.  $\Phi_{a/c}$  is fixed for a given ion species and substrate material and is assumed not to vary with the acceleration energy or dose. Furthermore,  $d_a$  is insensitive to the finer details of the tail parts of the distribution, so if the distribution is approximated with a Gaussian



Figure 13 Explanation of through dose  $\Phi_{a_{lc}}$ .

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function, we obtain

$$\Phi_{\mathscr{H}} \approx \int_{d_a}^{\infty} \frac{\Phi}{\sqrt{2\pi} \Delta R_p} \exp\left[-\frac{\left(x - R_p\right)^2}{2\Delta R_p^2}\right] dx$$
$$= \frac{\Phi}{2} erfc \left(\frac{d_a - R_p}{\sqrt{2\Delta R_p}}\right).$$
(26)

Hence, the analytical model of amorphous layer thickness  $d_a$  becomes

$$d_{a} = \begin{cases} R_{p} + \sqrt{2}\Delta R_{p} \operatorname{erfc}^{-1} \left( \frac{2\Phi_{a_{\ell}}}{\Phi} \right) & \text{for } \Phi \geq 2\Phi_{\gamma_{\ell}} \\ 0 & \text{for } \Phi < 2\Phi_{\gamma_{\ell}} \end{cases} (27)$$

As shown in **Figure 14**, by using  $\Phi_{a/c}$  which remains constant regardless of the implantation energy and dose, this model can predict the amorphous layer thickness with high precision. Thus, the simple addition of parameter  $\Phi_{a/c}$  in a database of ion implantation profiles lets us evaluate the thicknesses of amorphous layers formed under the wide range of conditions covered by the ion implantation database. So far, this theory has been applied to ion implantation in Si and Ge substrates and has produced highly accurate results.<sup>17)-19)</sup>



Figure 14 Comparison of theoretical and experimental amorphous layer thicknesses.

## 6. Conclusion

We have shown that our tail function is useful for constructing large-scale databases, and we have constructed an actual database based on this function. By adding parameter  $\Phi_{a/c}$ , defined as the dose of the distribution deeper than the thickness of the amorphous layer, and by linking this parameter to the ion implantation database, we made it possible to predict the amorphous layer thicknesses for a wide range of conditions. A system for predicting ion implantation profiles and amorphous layer thicknesses has been licensed to Mizuho Information & Research Institute, Inc. and has been made commercially available as the FabMeister-IM.<sup>20</sup>

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