

# Intelligent Material Design System based on Weak Conditioned Linear Programming

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## Abstract

*In recent year, multi-layered semiconductor package is one of the most important technologies to enhance its performance. To bond between each layer of multi-chip package, die-bonding film is known as an effective material. We had developed a novel low-modulus die-bonding adhesive film. Properties of the films are widely changed by the ratio of epoxy resin and acrylic polymer contents. To satisfy the target properties, the influence of various parameters on material properties was examined. However, it is not easy for researchers to find out the formulation which satisfy the targets. To solve the problem, this paper proposes the weak conditioned combinatorial linear programming method (WCCLP). By defining solution area as a function of combination index, the optimum formulations are acquired. This optimization can be done by newly developed user-friendly software. The software is applicable not only to semiconductor related materials but also to any such formulation as paint, medicine and food.*

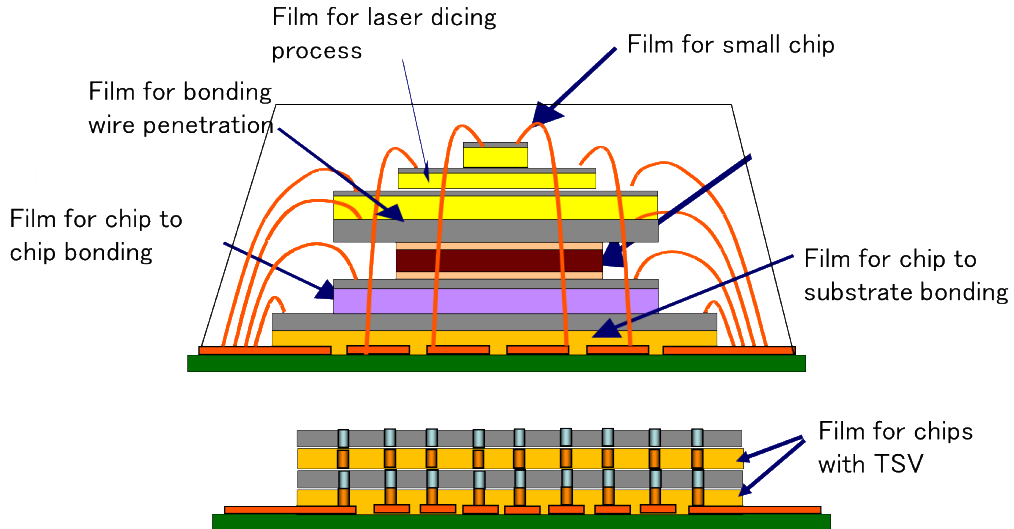
**Keywords:** *Material Informatics, Material Design, Die-bonding film, Linear programming, Search, Material blending analysis system*

## 1. Introduction

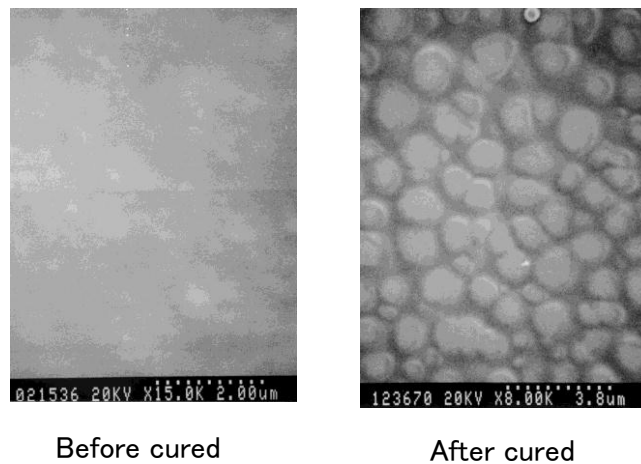
Recently, the advancement in electronic equipment demands more compact, lightweight and superior functional components. In order to meet with such intricate requirements, the mounting density per unit area has to be increased with new packaging methods using high performance materials. For example, in semiconductor packaging, the number of die layers is asked to be increased as shown in Figure 1, so that several kinds of die-bonding films are required to satisfy the requirement for high adhesive strength, heat resistance and resistance to thermal shock and so on. Epoxy resins have been widely used in microelectronics devices to achieve different functionalities. Epoxy resins coupled with rubber and proper curing agent can show desirable properties during mounting and in service with increased reliability. It has been shown that the reaction-induced phase decomposition [1, 2] of acrylic rubber/epoxy system results in improved thermo-mechanical properties. The morphology of rubber/epoxy blends can be well controlled to achieve desirable properties [3, 4]. The final morphology of the cured system depends on the competition between the cross-linking reaction and phase decomposition during curing. So it is desirable to control these two processes by varying the amount of rubber/epoxy ratio, type and amount of curing agent and optimum cure condition to achieve the desired phase morphology. Especially, rubber-matrix systems (Figure 2) show

the higher flexibility to thermal stress during the heat cycle compared with epoxy-matrix systems. To meet with the above mentioned requirements, we chose rubber-matrix epoxy adhesive for the development of new die-bonding film.

Properties of the films are widely changed by the ratio of epoxy resin and acrylic polymer contents. To optimize the properties of the die-bonding films, the influence of various parameters was examined by using the weak conditioned combinatorial linear programming which is our original mathematical design system [5-7]. By defining solution area as a function of combination index, optimum epoxy resin content, filler content etc. can be acquired. This optimization method can be done by newly developed user-friendly software.



**Figure 1. Application of Die-bonding Film in 3D Semiconductor Package**



**Figure 2. Scanning Electron Micrographs of the Surface of the Epoxy/acrylic Polymer Alloy Film**

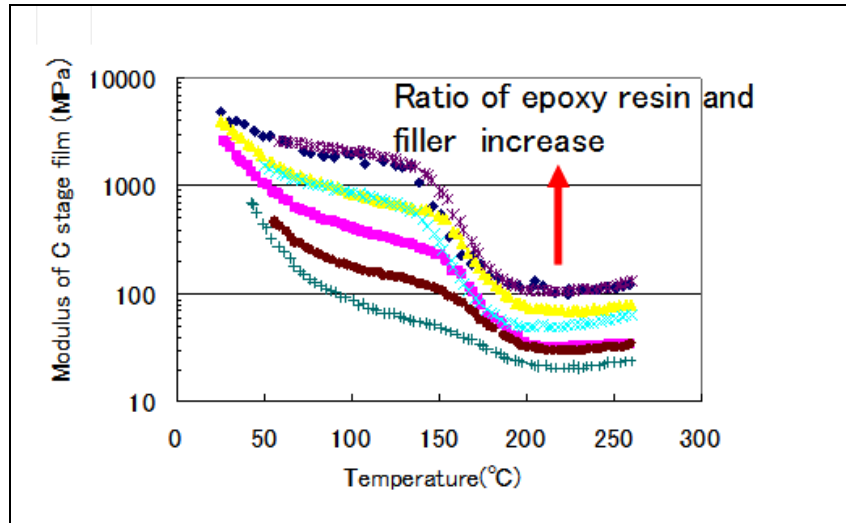


Figure 3. Modulus of the Die-bonding Film with Various Rubber/epoxy Ratio and Filler Amount

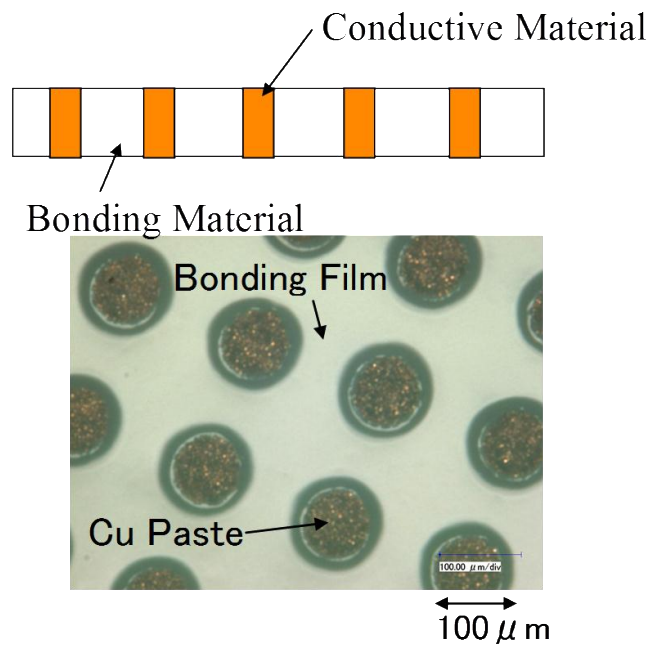


Figure 4. Die-bonding Film for TSV Application, Cross-section and Surface

## 2. Sample and System

### 2.1 A Die Bonding Film

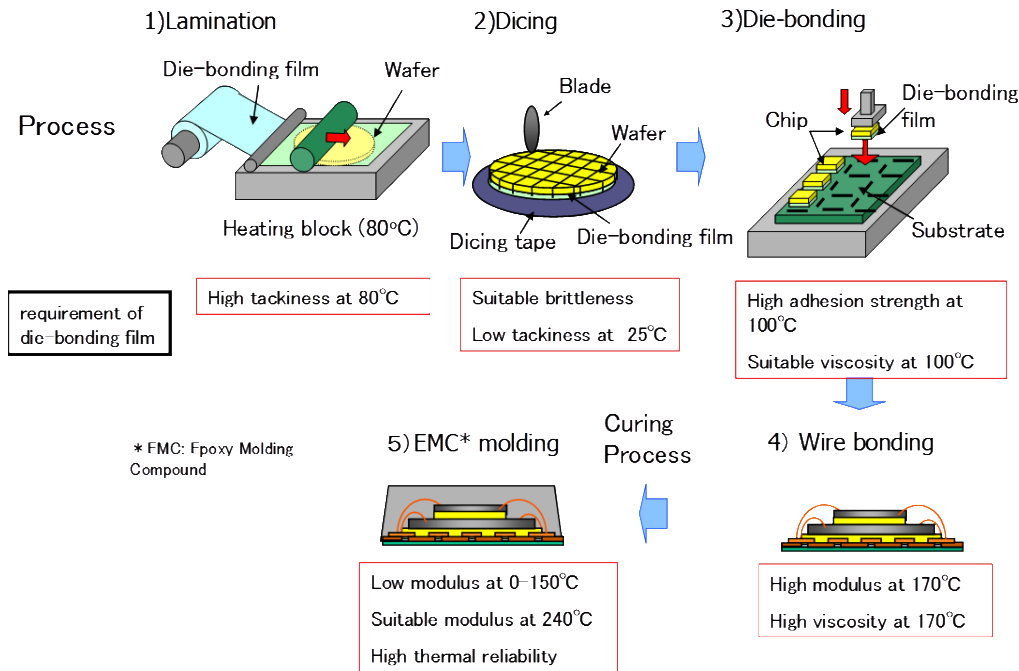
The varnish that consists of the copolymerized acrylic polymer which is a random copolymer consisting of acrylonitrile and several kinds of methacryl and acryl ether, epoxy resin (bi-functional and multi-functional epoxy resin), curing agent, catalyst and

the several kinds of inorganic fillers is coated on PET (poly(ethylene terephthalate)) film. The varnish is heated to get B stage (semi-cured condition) die-bonding film. Thickness of the film is 5-75  $\mu\text{m}$ . The modulus of film is widely controlled by varying the amount of rubber/epoxy ratio and filler amount (Figure 3).

For the TSV application, we prepare the die-bonding film with small hole in which copper conductive past is stuffed. The structure and surface appearance of the film is shown in Figure 4. The Manufacturing process of stacked CSP and the requirement for die-bonding film are shown in Figure 5. As shown in the figure, many kinds of properties are needed.

## 2.2 System for property optimization

The die-bonding film is needed to have not only enough adhesive strength but also the optimum life, tackiness, flow, heat resistance, etc. as shown in Figure 5. The optimization of all the properties by modifying chemical formulation is not easy because of the tradeoff relationship as shown in Figure 6.



**Figure 5. Manufacturing Process of Stacked CSP and Requirement of Die-bonding Film**

Linear programming (LP) [8] is well-known method to find the maximum or minimum of objective function under the given constraint and non-negative restriction. For example, the polygon is defined as the solution of simultaneous inequalities in xy plane. The contact point of such polygon and given minimization or maximization function is the optimum solution. The general expression of LP is shown in equations (1)

$$\left. \begin{aligned} f &= c^T x \\ Ax &= b \\ x &\geq 0 \end{aligned} \right\} (1)$$

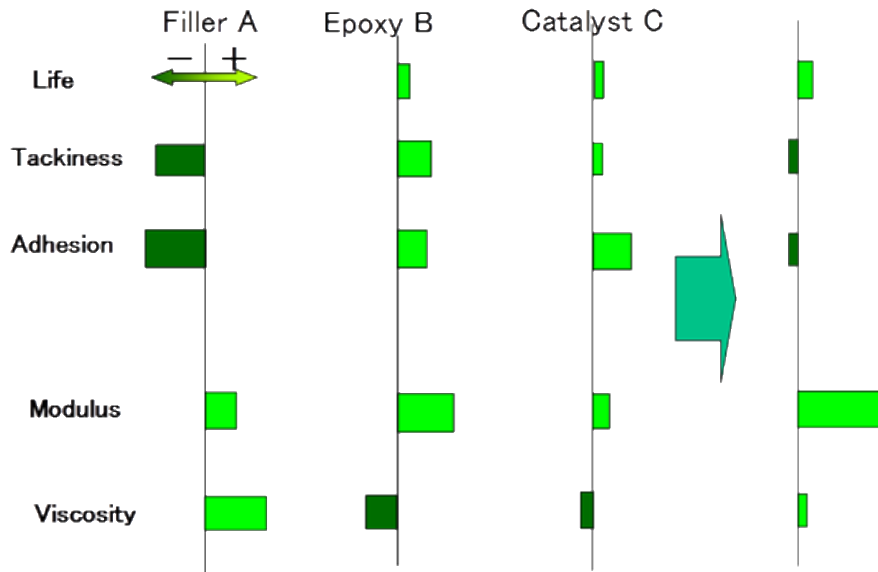
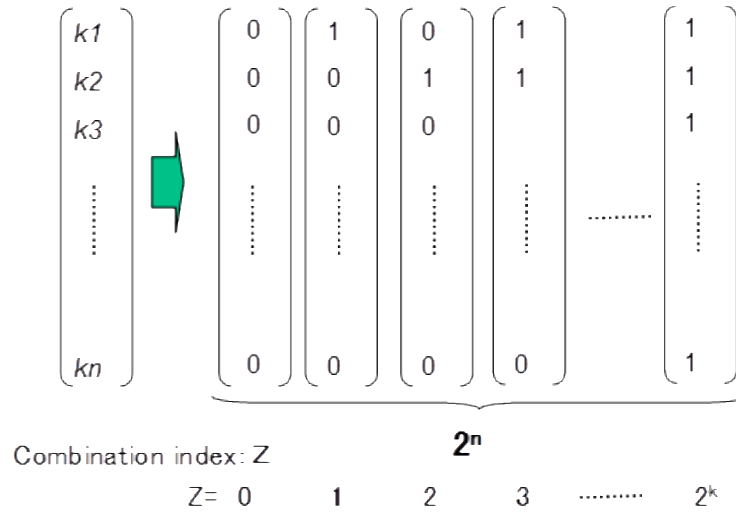


Figure 6. Example of Trade Off Relationship of Chemical Formulation

Table 1. General Representation of Matrix that show Correlation between Properties, Combination Parameter and Material's Parameter

Vector of properties	Properties/composition matrix	Combination coefficient	Vector of composition
$\begin{pmatrix} P1 \\ P2 \\ \vdots \\ Pm \end{pmatrix}$	$\begin{pmatrix} A11 & A12 & \dots & A1n \\ A21 & A22 & \dots & A2n \\ \vdots & \vdots & & \vdots \\ Am1 & Am2 & \dots & Amn \end{pmatrix}$	$\begin{pmatrix} k1 & C1 \\ k2 & C2 \\ k3 & C3 \\ \vdots & \vdots \\ kn & Cn \end{pmatrix}$	$\begin{pmatrix} C1 \\ C2 \\ C3 \\ \vdots \\ Cn \end{pmatrix}$

**Table 2. General Representation of Combinatorial Scalar Series and Combination Index**



In equation (1),  $A \in R^{m \times n}$ ,  $x \in R^n$ ,  $b \in R^m$ , and  $c \in R^n$ .  $A$  is coefficient matrix,  $b$  is right-hand matrix and  $c$  is cost coefficient vector.

For the material design application, LP is not always applicable. General extension of LP is necessary for this application because of the following reasons.

1) In the material design application, elements of  $x$  can be the amount of raw material (formulation) and conditions (intensity of physical procedure). The amount of raw material is non-negative value. The condition (intensity of physical procedure) is not always regular value. It can be negative value.

2) Some of the properties like dielectric constant, dynamic elastic modulus and specific heat capacity are defined as complex number.

3) The value of formulation and condition for process can be defined not only by unique value but also area. The minimization or maximization function is not necessarily defined by unique line or plane. It is defined as convex manifold which contains the minimization or maximization function.

4) Maximum number of raw materials is restricted for the production facilities and risk of raw material acquisition difficulty.

In this paper, we propose the weak conditioned combinatorial linear programming method (WCCLP) which is based on the linear programming method, which gives many kinds of improvement for the formulation and properties design. It can be said the extension of LP for materials design application. WCCLP is the method to alternate the proficient engineer's knowledge and intuition. This optimization can be done by newly developed user-friendly software.

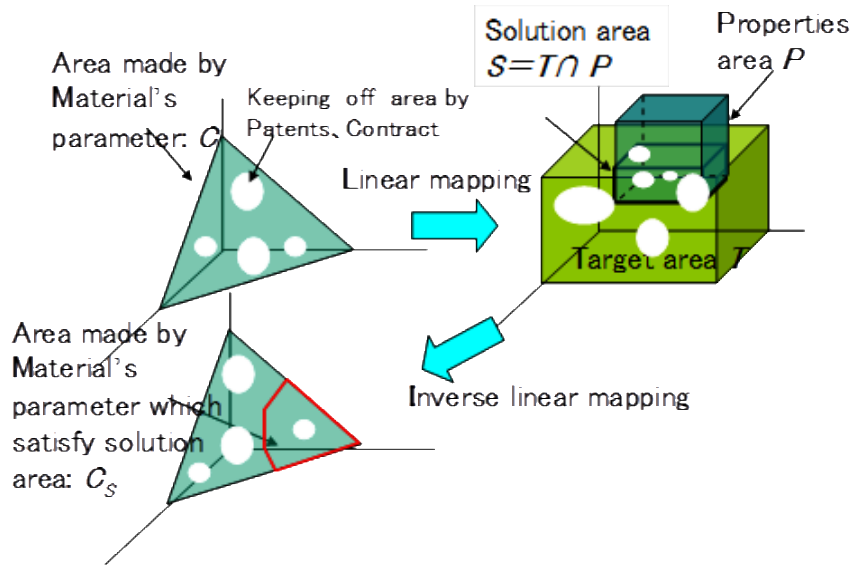
General expression of WCCLP is shown in equation (2). Vector  $x$  is amount of raw materials and physical procedures. Any elements of  $x$  which is variable vector can be regular or negative.

$$\left. \begin{aligned}
 f &= c^T \begin{pmatrix} x \\ y \end{pmatrix} \\
 A \begin{pmatrix} x \\ y \end{pmatrix} &= \begin{pmatrix} b \\ d \end{pmatrix} \\
 x_i &= [p_i, q_i] \\
 y_j &= [p_j, q_j] \\
 b_i &= [r_i, s_i] \\
 d_j &= [r_j, s_j] \\
 x &\geq 0 \\
 y &: \text{free}
 \end{aligned} \right\} \quad (2)$$

Some of the film properties like modulus and dielectric constant are expressed by complex number. So, all the vector and mapping between them should be defined in n-dimensional complex vector space. Matrix which maps vector of composition to vector of properties is acquired by many test results which are saved in the intelligent data base [5]. By applying this data base, the time of acquiring test results by many experiment is shorten.

If maximum number of raw materials was restricted, the combination coefficient and combination index should be defined in the matrix (Table 1). The combination coefficient is 1, if the raw materials or physical processing is candidate of formulation or process, and 0 corresponds to “not candidate”. The combination of raw materials or physical processing is defined as series of combination coefficient like 011010010..... and is rewritten as decimal number  $Z$ . The number of vector in solution set(S) is defined as a function of  $Z$  like  $S(Z)$  and  $\sum S(Z)(Z=0 \text{ to } 2^n)$  is the total solution set.

In Figure 7 the mathematical representation of solution area and mapping are shown. One composition vector is mapped properties vector space and if it is in the requested property set, the composition is in the solution set. These series of vector space are defined by the combination coefficient as shown in Table 2. Number of vector in solution set is defined as a function of  $Z$  like  $S(Z)$  and  $\sum S(Z)(Z=0 \text{ to } 2^n)$  is total solution set.



**Figure 7. General Representation of Solution Area and Mapping Defined by Matrix that Show Correlation between Properties and Material's Parameter**

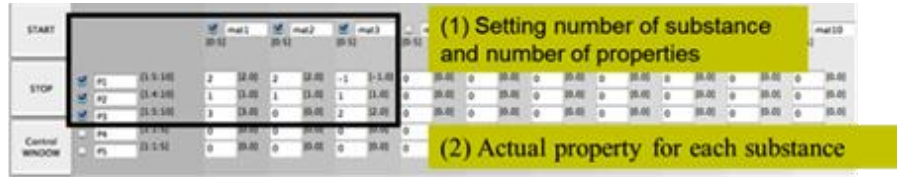
### 3. Results and Discussion

All the procedures and calculation can be done by newly developed user-friendly software which we have developed. We propose the practical system for the material engineer. By this system, materials design can be done without special knowledge of linear programming and algebraic verity. The proposed system consists of two systems.

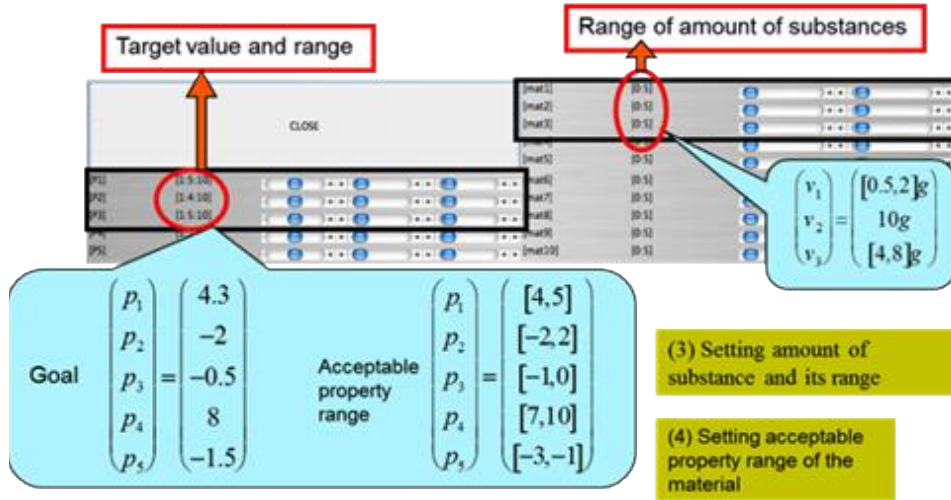
One is M-Designer's Goal Quest. The example of the interface is shown in Fig. 8. M-Designer's Goal Quest has the interface for input of the value of properties/composition matrix, target properties, maximum and minimum value of formulation contents and physical processing condition. User also can fix the prohibited value and upper and lower limit of formulation. The restrictions are economical, legal, patent restriction of amount of composition, etc. Then the system starts calculation and shows the results (all formulation which satisfy the target properties) by each combination index (Figure 8). The example of the obtained result is also shown in Figure 8. The formulations within the defined target area are shown firstly. Secondly, formulations which partially satisfy the defined target area are shown.

Among the various algorithms, such as the simplex method, the interior point method is frequently proposed in the conventional linear programming. But, these high speed solvers are not applicable for the system discussing in the paper. Because they treat concave polyhedron and taurus in complex vector space. In this paper, we adopted the simple calculation algorithm. Vector of properties space of discrete amount of vector of composition is calculated by each combination index. If vector of properties satisfies the target value, it is recorded as one of the solution. This system can't search optimum solution, but search solutions which satisfy the requested value, so calculation time is relatively short.





(a) Coefficient matrix



(b) Constrained condition

Figure 8. Initial Input by Users

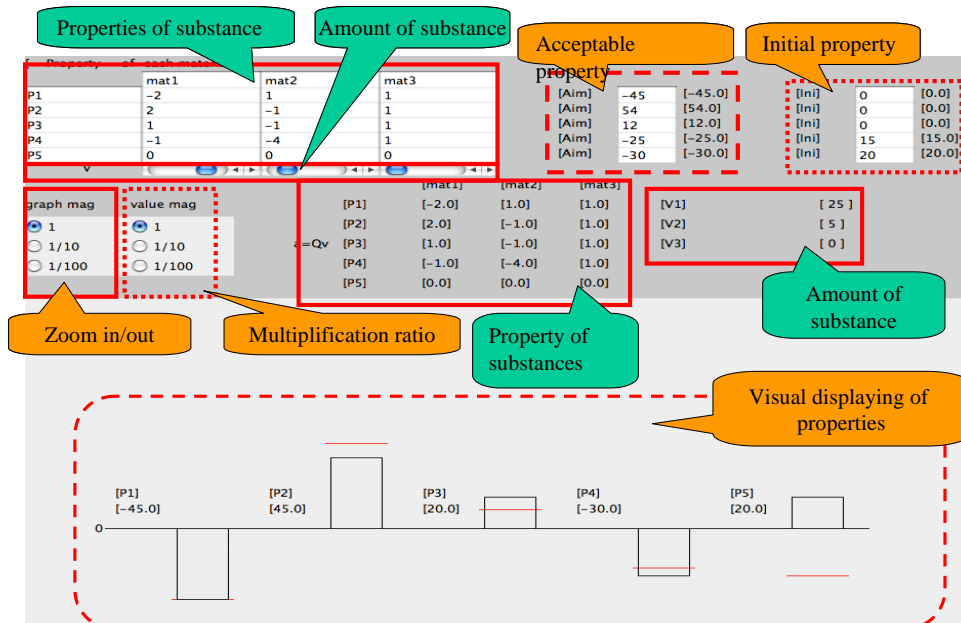


Figure 9. Example of M-Designer Viewer

The second one is M-Designer's Viewer. By this system, solutions calculated by M-Designer's Goal Quest are shown as a list or map in 2 or 3 dimensions. Figure 9 is the interface for inputting the value and calculation execution of Designer's Viewer. In this window, the coefficient matrix and the value of targeted range are inputted. The relationship between target value range and the map of solution is visualized, and the margin or flexibility of the material formulation is grasped. Both systems are by Java as an applet. This system is applied for developing novel die-bonding film for 3D packages. The target value and restrictions are listed below.

$$\begin{aligned}
 P &\geq 1MPa \\
 E &\geq 280 \\
 r &\leq h \\
 s_i &\leq 8\%
 \end{aligned}$$

Vector of properties was calculated by properties / composition index listed below.

$$\begin{pmatrix} P+0.44 \\ E-430 \end{pmatrix} = \begin{pmatrix} 0.45 & 0.17 & 0.15 & 0.013 & 0 & 0 \\ -10 & -24 & -15 & -3.2 & -4.5 & -8.3 \end{pmatrix} \begin{pmatrix} k_1 & r \\ k_2 & s_1 \\ k_3 & s_2 \\ k_4 & s_3 \\ k_5 & s_4 \\ k_6 & s_5 \end{pmatrix}$$

Here,  $P$ : peel strength,  $E$ : modulus,  $k_i$ : scalar value,  $r$ : functional group content of acrylic rubber,  $s_i$ : silica. The diameters of the investigated silica fillers are  $s_1$ : 6 nm,  $s_2$ : 10-20 nm,  $s_3$ : 600 nm,  $s_4$ : 1900 nm and  $s_5$ : 4200 nm. One of the results is shown in Figure 10. The amount and diameter of inorganic filler and amount of functional group in acrylic polymer are parameter and requested value are peel strength and modulus of C-stage (cured) film at 240 °C. In Figure 10, the half of the mapped area satisfies the target value. The formulation which satisfies the requested properties is shown in Figure 11. The formulation is decided considering the deviation and margin. In this case, right area has large margin for the filler amount deviation.

We show the flow chart of this system in Figure 12. This system is applicable to the material which shows linear or semi-linear properties/composition relationship like acrylic / epoxy resin reaction-induced polymer alloy films. After finding the solution area, nonlinear calculation also can be done.

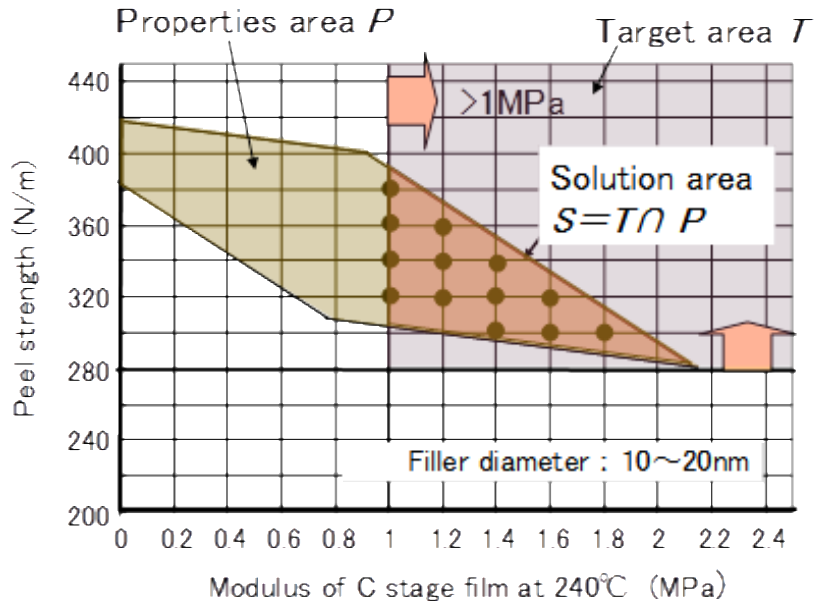


Figure 10. Example of Result of Computation of Target Properties Area

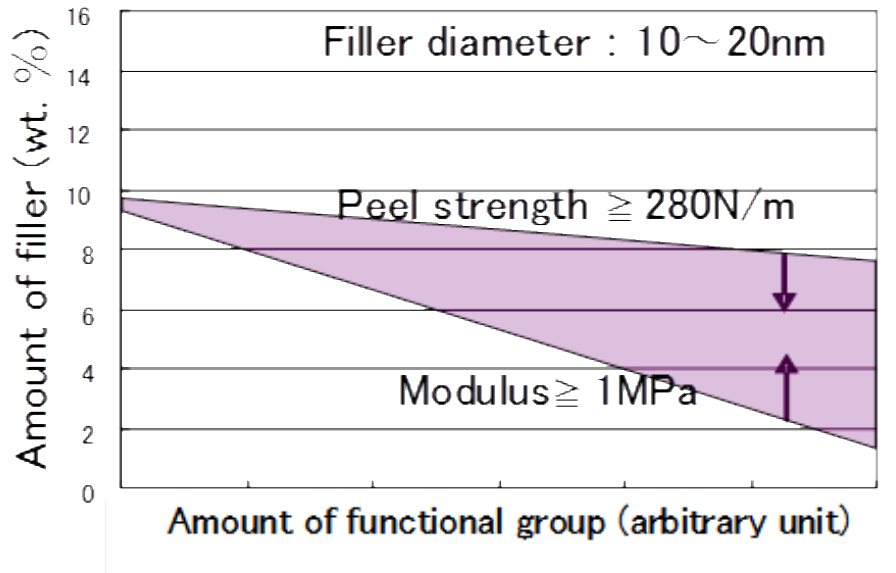
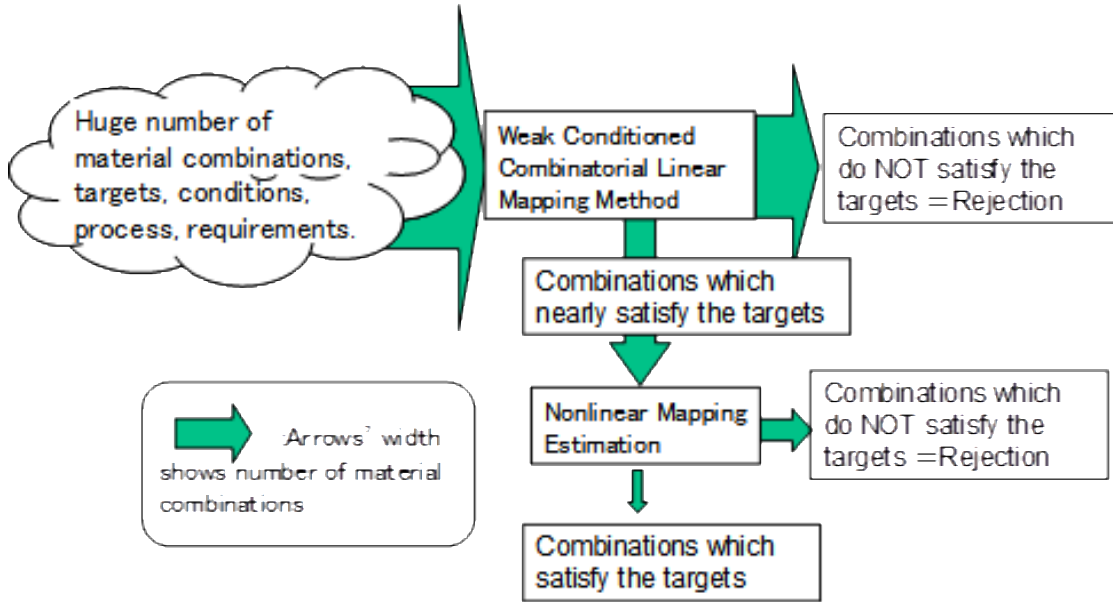


Figure 11. Example of Result of Computation of Optimum Formulation



**Figure 12. Flow Chart of Optimization Process by Weak Conditioned Combinatorial Linear Programming Method and Nonlinear Estimation**

#### 4. Conclusion

We proposed a new material design method (weak conditioned combinatorial linear programming method) that is based on the linear programming method. By applying this method, many kinds of properties can be changed and controlled at one time, saving the time for adjusting the properties of die-bonding film for 3D-packages. This method is effective to search the combination of a well-balanced material or the targeted value though accuracy cannot be pursued. We also developed user friendly software applicable not only to semiconductor related materials but also to formulations such as paint, medicine, food, etc.

The materials for 3D-packages necessitate not only very precise property control in each packaging production process, but also the excellent stability, thermal resistance and stress relaxation. The material development of various kinds of package based on the experience and intuition is becoming insufficient and outdated. We are pursuing the more effective and user friendly system to overcome the restriction of material of the linear relationship in the future.

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Dr. Inada graduated Tokyo institute of technology, department of textile and organic materials in 1988. After getting master degree in material science at Tokyo institute of technology, joined Hitachi Chemical Co. Ltd. in 1990. He got Ph.D. degree in material science at Yamagata University in 2007. His current research interest areas include material informatics, network polymer and mathematical approach for the material development.



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He has served a lot of conference/program/workshop chairs including ACIS SNPD 2009, 2012 and 2013; CAINE 2012; ACIS SSNE 2011; IEEE/ACIS ICIS 2010 and 2013; IEEE IWEA 2007-2011; IEEE CEC 2011 and 2012; IEEE PRIWEC 2006; IEEE/ACM/WIC ECBS 2008 and 2009; ACAN 2005-2012; and other 20 academic events. He has received over totally 40 awards and research grants from international conference, research foundations, companies and government. He has ever published over 300 research papers and articles in this decade. He is a member of IEEE, ACIS, IIAI, IEEJ, and several other academic societies.

He is current research interest areas include Tourism Informatics, Material Informatics, Safety Service for Disaster Recovery, Designs on Secure Electronic Commerce Systems and e-Auction Protocols, Career Service System, Qualitative Reasoning and Simulations. Some of his researches are presented in several top ranked international conferences including AAAI, IEEE CEC, AAMAS, and WW The main title (on the first page) should begin 1 3/16 inches (7 picas) from the top edge of the

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