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Materials Curation: A Tool for Drawing Material Design Principles

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Abstract: ***A tool is proposed for drawing materials design principles to help in accelerating the research and development of materials. This aims to help researchers to use alternatives to (sometimes) non-scientific customs or conventions in finely subdivided, narrow scientific fields. Instead, it enables the exploration of materials within broad, multidisciplinary fields based on the scientific principles of their function and performance with full utilization of the materials information available. Several examples are presented using this tool. Following this, the flowchart for drawing design principles with the tool, and its characteristic features are explained. The relationships and combinations of various types of materials quantities are considered based solely on the essential conditions from scientific principles, without reference to technical possibilities. These relationships and combinations between the different physical or chemical properties are used to create a connecting network using scientific principles. Materials search through various databases using informatics tools is required to suggest concrete materials that match these design principles. High throughput synthesis/analysis/theoretical calculations such as Density Functional Theory (DFT) calculations are necessary to optimize the materials suggested for practical applications.***

Keywords: material design, multidisciplinary, information, design tool, information network

1. Introduction

The increasing need for new materials to solve various social problems, such as resource and energy limitations, and the greenhouse effects, is being accompanied by acceleration in materials research, owing to rapid developments of experimental techniques, equipment (including combinatorial techniques), super computers, and packages for various theoretical calculations including first-principles DFT calculations. The Materials Genome Initiative (MGI) in USA [1] has been established under these conditions. MGI involves not only high-throughput experimental equipment and DFT calculations, but also information technology and computational tools for predictive modelling, simulation, design, and exploration. The demand for information technology and computational tools comes from the difficulty in finding and combining appropriate and useful information from the vast amount of data produced daily from various sources, such as experimental results, computer calculations, and scientific papers.

Predictive modelling, simulation, design, and exploration appear to be of particularly great importance owing to the following facts. First, if a "carpet bombing" approach is used, the number of trials required to find a material with a specific desired property becomes astronomical. How much time will be needed for this? In the periodic table, there are 76 elements that are of practical use (this excludes the inert gases, and elements without stable isotopes). For simplicity, assuming the variety of elemental species is 70 (instead of 76), the number of elements in a material is n, and searching for materials with concentration variations in 1 at% steps, the number of possible materials with different compositions is expressed as 70!/(70-n)!* 99!/(100-n)!. If one hundred materials can be synthesized, or calculated, per day in each laboratory using high-throughput experiments or DFT calculations, and there are one hundred laboratories, more than 5,600,000 years will be needed for 4-element systems (n=4), and approximately 360 million yeas for 5-element systems (n=5). A further complicating factor is that material variations with compositional gradients, layers with different compositions (such as super-lattices), and nano-structured materials will also exist. Therefore, even when utilizing high-throughput techniques, "carpet bombing" without predictive modelling, simulation, and design is unrealistic. The other fact is that a considerable number of materials in practical use, especially for structural applications, are polycrystalline or mixtures of different phases; here, sequential multiscale modelling from atomic scale to grain size, and subsequently, to real size is required. For example, Ferrium® S53 steel, corrosion-resistant landing-gear steel, has been developed by multiscale computer design by Prof. Olson‟s group at Northwestern University [2].

With functional materials, such as electronic materials, magnets, and catalysts, their properties are mostly determined by the constituent materials, such that multiscale considerations are not too critical. However, for these kinds of materials, the varieties of elemental combinations are huge, and materials with unexpected elemental combinations are sometimes discovered. Because of these problems, a brief concept of a new tool to draw design principles has been proposed [3]. This can help researchers to use alternatives to custom or conventional methods (which are often non-scientific) in finely subdivided, narrow scientific fields, and explore materials from wide, multidisciplinary areas, based on scientific principles of function performance, with full utilization of available materials information. In this article, some examples on drawing design principles using this tool are demonstrated. The fundamental features, that are common among the examples, are presented as the characteristics of this new tool.

In the contemporary specialized and subdivided world, multidisciplinary combinations of existing knowledge or information can provide solutions or provide new valuable insights. Presenting such a valuable insights produced by combinations is called "curation", especially in business-related fields [4]. Because of the similarity to content handling, the tool presented here is called “materials curation”. Materials curation does not pin-point the structure or chemical composition of materials needed for a particular use, but, rather, gives a guideline, or design principle, for searching for potential materials. Once the guideline is set, one can find a target material by utilizing high-throughput methods and informatics.

2. Examples of Design Principles by Combining Knowledge from Different Fields

2.1 Tuning work function by mixing two metals

The first example is a guideline for work function tuning in electronic devices. In many electronic devices such as diodes and transistors, it is known that the Schottky barrier height (SBH) and operation voltage are determined by the work function of an electrode material (φm). Researchers in device materials have been using a trial and error approach to tune work function, either by mixing two metals with different work functions, or by making layers of metals with different work functions. However, when the origin of work function is considered from a surface physical point of view, and the phase diagram pattern in binary systems from a metallurgical point of view, a guiding principle for work function tuning can be extracted [5], which is briefly explained below. At first, by which quantities work function is determined should be understood. In a surface physics textbook, a relationship between work function and Wigner-Seitz cell radius (= valence electron density, which is determined by the number of valence electrons and the lattice constant) is found for the most simple case. Therefore, the change of valence electron density with composition is examined in the phase diagram and the number of electrons in each phase. The process of extracting the guiding principle is shown in figure 1(a). Knowledge/information from three different fields is combined: the operation voltage of a device is determined by the work function of the electrode metal; several experimental results on the relationship between work function and composition in binary systems reported in the surface physics field can be explained by the types of phase diagrams corresponding to the binary systems. There are two important facts, which are well known in surface science, but not in the device material field. One is that simple mixing of a low-work-function metal with a high-work-function one does not always produce a material with an intermediate work function corresponding to the composition. The other is that making a layer with metals of different work functions is not effective for tuning the work function, unless the metals diffuse and form a new material. The relationship, thus obtained, between the work function and phase diagram, as a function of composition, is shown in figure 1(b). A detailed discussion of the relationship is given in ref. 5.

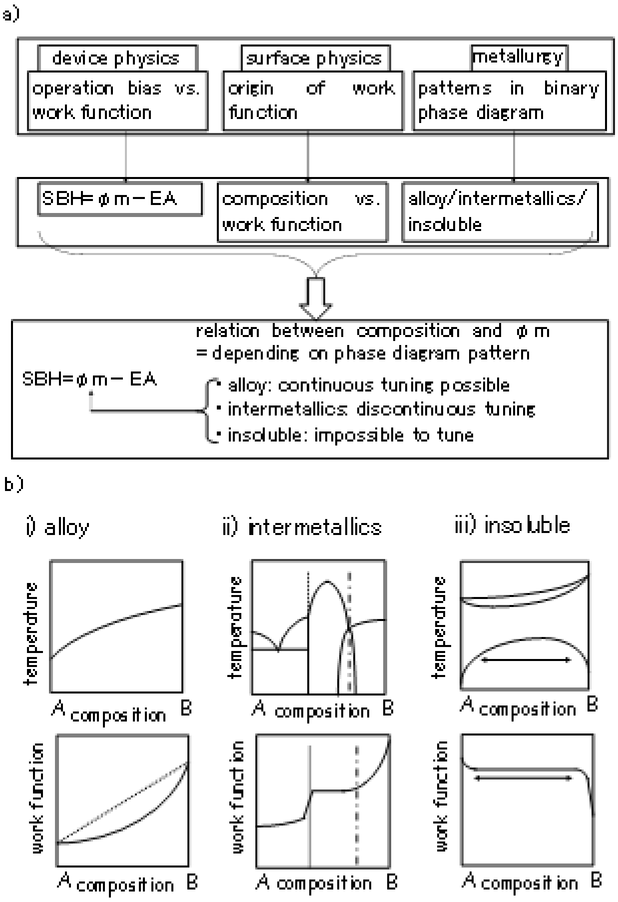


Figure 1: (a) A scheme to draw a guideline to tune work function by mixing two metals. The relationship between Schottky barrier height and work function of metal in device physics emphasizes the need for tuning work functions of metals for electrical device development. In surface physics, the origin of the work function is known, and some experimental results on work function modification as a function of chemical composition in binary systems have been reported. Different types of phase diagrams are known in binary systems in the metallurgy field. Hence, the chemical composition of binary systems is not always the ratio of mixed metals. Combining this knowledge provides the guide to mixing two metals for work function tuning, which depends on the type of the phase diagram of metals mixed. (b) Schematic representation of work function modification as a function of chemical composition according to different types of phase diagrams. For two metals A and B, which form a solid solution, the work function changes continuously according to the chemical composition, although not linearly. It is concave in most cases (i). When A and B form an intermetallic compound, the work function stays nearly constant for a composition range of the compound, but suddenly changes at the edge of the composition (ii), because the atomic and electron density change drastically at the phase boundaries. In case A and B do not mix (miscibility gap in the phase diagram), the work function value is nearly constant for most of compositions and close to the value of the metal with a lower melting point.

In this example, random mixing of a low-work function metal with a high-work function one for tuning of the work function in electronic devices is systemized based on the design principle for mixing, which is derived by combining knowledge in surface physics and metallurgy with that in device physics.

2.2 Thermoelectric materials with high figure of merit

The second example is finding a new category of materials with a high figure of merit for thermoelectric materials. A value of the figure of merit is described by $S^2\cdot\sigma/\kappa$, where S is the Seebeck coefficient, σ is the electric conductivity, and κ is the thermal conductivity. Two approaches, finding materials with high Seebeck coefficient and/or finding a way to reduce thermal conductivity, are in the main stream in the development of thermoelectric materials. Because both the Seebeck coefficient and electric conductivity are affected by the carrier density, but in the opposite sense, materials search is usually focused on a high Seebeck coefficient rather than high electric conductivity. Most researches for high Seebeck coefficient involve the modification of chemical components in previously studied materials. The main method to reduce thermal conductivity is to fabricate nanostructures. In the “materials curation” tool, the physical basis of the three parameters is first examined. The physical origin of the thermoelectric effect is the change in electronic energy distribution with temperature, resulting in the shift of the Fermi level (chemical potential). This change is well known as the Fermi distribution function [6]. Therefore, once the density of states (DOS) of a material is known, we can obtain both thermoelectric power, without considering electron diffusion (V“), and temperature differentiation of V“, S“=dV“/dT, called the quasi-Seebeck coefficient. Although the Seebeck coefficient is the derivative of thermoelectric power with temperature, considering electron diffusion, S“ is used as a measure of the Seebeck coefficient to decouple it from electric conductivity. The electron conductivity is proportional to carrier density and mobility, where the latter is independent of the Seebeck coefficient, and is inversely proportional to effective mass. Therefore, we look for materials with a small effective mass. Although not many experimental values have been reported for effective mass, a hint can be obtained from electronic band structures, because the inverse of effective mass is proportional to (dE^2/d^2k), where E is the electronic energy and k is the wave number of the electrons. After screening materials with S“ from DOS and effective mass from electronic band structure, electric conductivity can be tuned by doping. With the thermal conductivity, lattice thermal conductivity contributes mainly due to smaller electronic thermal conductivity in thermoelectric materials (non-metallic). To reduce lattice thermal conductivity without decreasing electric conductivity, it is preferable that the number of atoms in a unit cell or the molecular weight of a unit cell is large, or a particle ensemble is made with a nanometre-sized gap. For this reason, researchers have searched for materials such as clathrates and skutterudites (natural nanostructured materials), or tried to fabricate artificial nanostructures. A new category of materials with a high figure of merit can, therefore, be explored using the information on DOS, electronic band structure, and unit cell size or molecular weight. The above process of materials design is shown schematically in figure 2(a). In this case, the first important point is that the Seebeck coefficient indicator is decoupled from electric conductivity by utilizing knowledge on the temperature dependence of chemical potential in semi-conductors; hence, this indicator is calculated solely from the DOS and the Fermi distribution function. The shape of DOS appropriate for high Seebeck coefficients as n-type thermoelectric materials for a certain temperature range (determined by the band gap Eg) is shown in figure 2(b).

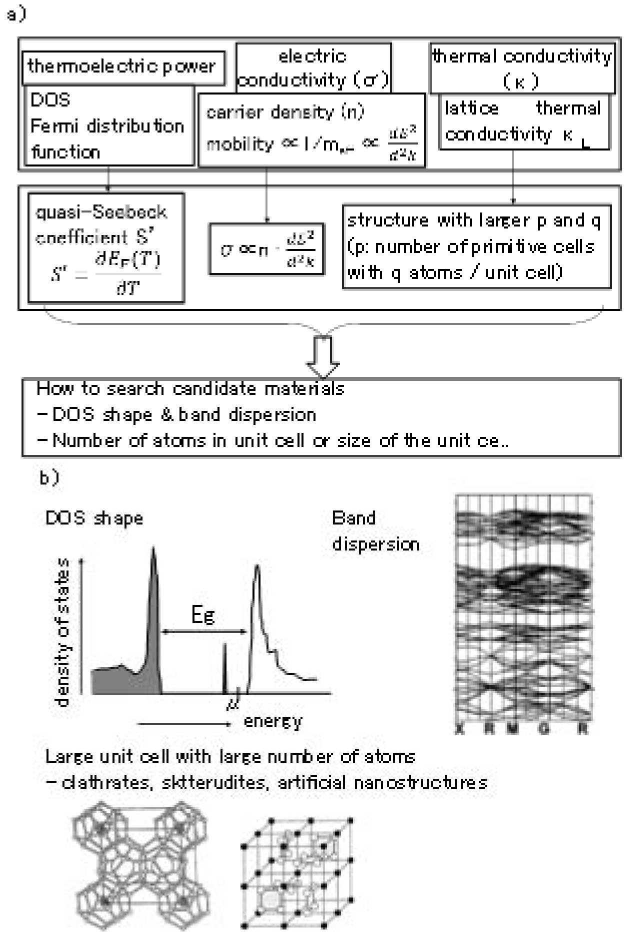


Figure 2: (a) A scheme to obtain a guide for finding materials with high figure of merit, which is determined by Seebeck coefficient, electric conductivity, and thermal conductivity of the materials. Because the Seebeck coefficient is influenced by electric conductivity, the quasi-Seebeck coefficient that does not take the diffusion of the carrier into account is used instead. The quasi-Seebeck coefficient can be calculated simply from the density of states of the material and Fermi distribution function without considering electric conductivity. Electric conductivity is proportional to carrier density and mobility of the carrier. Because carrier density influences the Seebeck coefficient, the mobility should be explored, which is proportional to (dE^2/d^2k), whose value can be obtained from band dispersion. Regarding thermal conductivity, only lattice thermal conductivity is an independent parameter, since electric thermal conductivity is a function of electric conductivity. Small lattice thermal conductivity can be obtained by a lattice with atoms that scatter large amounts of heat without preventing electric conductivity, which means a large unit cell and/or unit cell with large molecular number. (b) Information for searching for materials with high figure of merit deduced using figure 2(a).

Practical thermoelectric materials, such as BiTe and PbSb, have DOS shapes similar to that in figure 2(b). The second point is that electric conductivity is divided into carrier density and mobility, so that materials design is possible via information on mobility without considering the Seebeck coefficient directly. From the electronic band structure, such as that shown in figure 2(b), the value of (dE/dk) can be estimated from the gradient of curves near the Fermi level; then, the mobility can be obtained, which is proportional to (dE^2/d^2k). The third point is that a search based on thermal conductivity, which is a physical property, can be conducted using structural parameters, such as unit cell (number of atoms in a unit cell is large) and molecular weight. Examples of structures that have a large unit cell are shown in figure 2(b).

The advantage of the guiding principle in this example for materials search is that DOS, band structure and crystallographic structural data, which are reported both in the thermoelectric research field, and in various application ones, are available. It is expected that searching for materials with a DOS shape similar to that in figure 2(b), which has not yet been explored from a thermoelectric point of view, is a promising way to find a new category of materials with a high figure of merit. [7] Unfortunately, the numerical DOS data available are limited to some simple, pure materials. Most of the DOS data are in graphical form, and cannot be handled numerically by a computer. Therefore, one has to check DOS figures by hand, one at a time. Although efficient search by hand is impossible, a couple of candidate materials have found by the author, β-HfNCl [8] (from super-conductor research) and $LuFe_2O_4$ [9] (from giant magnetocapacitance research). Screening of potential materials by the size of unit cell or molecular weight of unit cell will be also effective to find a natural, low heat conductive material.

In this example, the so-called trade-off relationship between S and σ, via electron density, has been decoupled as a consequence of the origin of thermos-electric power (solid state physics), and the relationship between electric conductivity and DOS modification by doping (device physics). The resulting design principle involves seeing the DOS shape for high thermos-electric power, to find a value of (dE/dk) to provide high carrier mobility, and to dope until the appropriate electric conductivity is obtained. Furthermore, the design principle for low κ involving screening materials by unit size, number of atoms in a unit cell, and/or molecular weight of a unit cell, adds to the known principles for making artificial nanostructures.

2.3 A substrate suitable for the growth of atomically flat epitaxial thin films

The third example is more specific than the previous two ones. During a study on the interface between metal and alumina as a model system for high-k gate material for a future CMOS, the author tried to find an appropriate metal substrate for the growth of atomically flat, ultra-thin, epitaxial alumina films. This example shows how the substrate metal has been found using the proposed tool.

An initial reading of references about epitaxial alumina film growth, either atomically flat or rough ones, led to the following insights. When epitaxial alumina was grown on pure metals, such as Mo and Ta, aluminium metal was initially deposited on the substrate, and then it was annealed in an oxygen atmosphere. The alumina film grew as very rough islands. In contrast, when Al-containing metal systems, such as NiAl and FeAl, were used as substrates, atomically flat, epitaxial alumina films grew by oxidation of the substrate. The following conclusion was made about the mechanism of differences in the growth mode: When oxygen is introduced into the system, many aluminium atoms try to bind with oxygen due to the high thermodynamic stability of Al-O bonding on Al-deposited surface. This aggregation of aluminium atoms is the origin of rough alumina formation. However, on the Al-containing metals, aluminium atoms are separated by the other element in the lattice. When oxygen is introduced, oxygen atoms adsorb on aluminium atoms without aluminium aggregation. The first flat layer is formed in this way, with Al-O bonding. In order to grow the second layer, further aluminium atoms have to be supplied from the bulk of the substrate. Because the positions of oxygen atoms are fixed on the surface, due to the Al-O bonding already present, the newly supplied aluminium atoms bind with the oxygen atoms on the surface, which the capture oxygen atoms from the atmosphere immediately after reaching on the surface. Since the oxygen-adsorbed surface does not catch additional oxygen atoms from the atmosphere, the growth process proceeds like atomic layer deposition. Therefore, an atomically flat alumina film is formed (figure 3(a)).

Although atomically flat alumina film formation has been reported with Al-containing metals, the thickness of the films reported never exceeds 1 nm, which is essential for the use of the films as gate insulators. The explanation can be obtained using estimates from the author‟s reflection high energy electron diffraction study on the growth of thick alumina layers on NiAl (110) [10]. On the NiAl (110) surface, the growth of flat alumina film usually stops at 0.5-nm thickness. In this study, an increase in the thickness of the flat alumina film was achieved by repeating Al deposition and oxygen introduction on 0.5-nm-thick flat alumina film. However, the crystal structure of the alumina film changed as it grew thicker, and turned into a polycrystalline one, due to the stress in the film. This study suggests that crystallographic symmetry and lattice matching is important for thick film growth, as is already known in the field of hetero-epitaxial film growth of semiconductors [11]. All flat alumina films grew with 6-hold symmetry on the surface, with oxygen atoms in a closed pack manner.

From the above discussion, it can be concluded that Al-containing metals with 6-hold symmetry on the surface should be searched for, whose lattice constant matches that of alumina. It should be noted that all the Al-containing metals studied so far were intermetallic compounds, such as NiAl and FeAl, in which the atomic arrangement in the lattice is similar to body-centred cubic, with no 6-hold symmetry. Usually, intermetallic compounds have rather complicated crystal structures and not many have crystal planes with 6-hold symmetry. Therefore, alloying Al to pure metals (making solid solution) that have 6-hold symmetry must be considered. The crystal structures that have planes with 6-hold symmetry are either face-centred cubic or hexagonal closed-packed structures. By examining the crystal structure, lattice constant of pure metals, and solubility of Al, several candidates for a substrate were found (figure 3(b)). For practical use, expensive or rare metals were excluded [12]. As a result, the Cu-Al alloy (111) surface was selected as a candidate. The single crystal of the alloy was made to order by a company. We successfully grew flat alumina films of more than 1-nm thickness [13], as anticipated. The films showed high stability and very good insulating properties [14], appropriate for a model interface of a high-k dielectric gate and gate metal. Following our success in the growth of flat alumina films, this alloy is now commercially available, with many orders from international laboratories. In this example, the basic principles of growing flat layers are already known, and introduction of stress by the mismatch of symmetry and/or lattice constant during the film growth is also established. However, by combining these two areas of knowledge for the growth of flat epitaxial alumina films, which had not previously been attempted, a suitable substrate for atomically flat epitaxial thin alumina films was found.

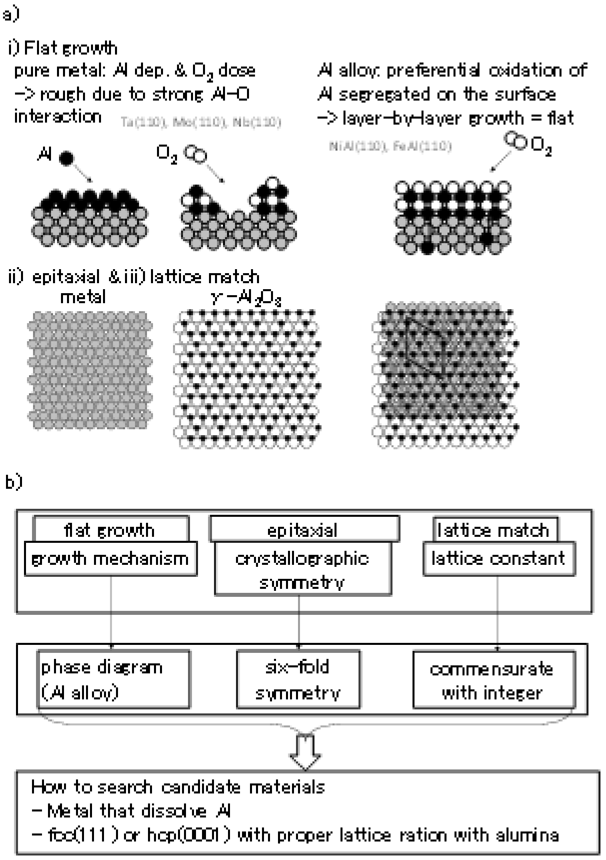
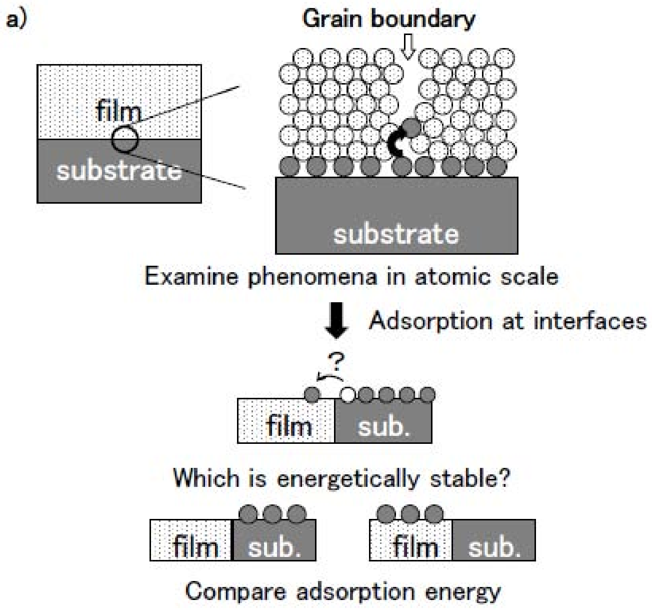


Figure 3: (a) The scientific reason for the difference in the growth mode of alumina film deduced from references (i) and crystallographic conditions for epitaxial growth (ii). (b) A scheme to obtain a guide for finding materials appropriate for the growth substrate of atomically flat, thin epitaxial alumina films. Three main factors can be extracted from literature references: the method for growing atomically flat films, symmetry matching of the substrate with alumina films, and lattice size matching.

2.4 Surface Segregation of Under-Layer Elements

The final example involves a generic prediction method, which the author developed of the surface segregation behaviour of under-layer elements in layered materials [15]. Before the method was developed, there had been many reports of observations of surface segregation of under-layer element, using Auger electron spectroscopy [16], Rutherford backscattering spectroscopy [17], etc. However, information about conditions of segregation was completely chaotic. The author conducted systematic experiments on surface segregation of under-layer metal in bimetal systems, and identified several important facts on the phenomenon [18]. These indicated that non-bulk properties control whether surface segregation occurs or not. We then had the idea of considering atomic movement at the interface between the under-layer and a layer above. If one imagines the thermal excitation of random atomic diffusion, migration of under-layer atoms on the grain boundaries of a layer should occur with some probability (figure 4(a)). If we consider that the migrated atoms do not return to the under-layer, when the adsorption energy on the grain boundary is larger than that on the under-layer (when atoms go back), this will result in the flow of atoms toward the surface along grain boundaries. From this consideration, the occurrence of segregation can be predicted by comparing the adsorption energy of the under-layer element on the film with that on the under-layer. This explains why the segregation behaviour has been reported to be dependent on the annealing atmosphere. A problem exists here: there is no library of adsorption energy data for any combinations of two materials. Experimentally measured values of adsorption energy are very limited. However, after a long search, at the time without any convenient internet searching systems, the author found a semi-empirical method for estimating adsorption energies that is generally usable. This was based on the mixing enthalpy of metals [19]. Now, the surface segregation problem in film technology can be predicted by combining adsorption energy of atoms in the surface chemistry field and mixing enthalpy in the metallurgy field (figure 4(b)). The surface segregation prediction method, constructed in this way, is now available on the web site for free use [20].



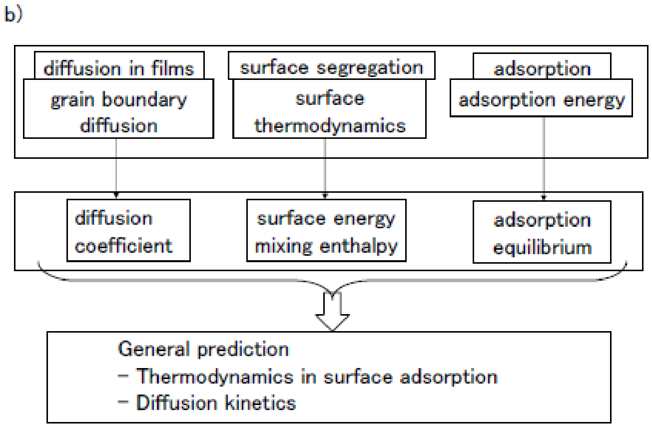


Figure 4: (a) The scientific reasoning on the factor that determines surface segregation of substrate atoms. From consideration of atom migration at substrate-film grain boundary and thermodynamic equilibrium in adsorption, the determining factor is found to be the adsorption energy of substrate atoms on either film element or substrate element. (b) Scheme to obtain a guide for predicting surface segregation of substrate atoms on the film and the substrate. Because substrate atoms appearing on the film surface diffuse through its grain boundaries, the diffusion coefficient is governed by grain boundary diffusion. However, the occurrence of surface segregation is governed by surface thermodynamics, which is determined by parameters such as surface energy and mixing enthalpy. The stability of grain boundary migration is governed by the thermodynamic absorption equilibrium determined by the adsorption energy.

2.5 Examples of discoveries likely made using a similar way of thinking

In this section, two discoveries are presented that the author feels were made using a similar method to this tool.

One is halogen perovskites for solar cells. The organic-inorganic perovskite (ABX_3 crystal structure) system, now regarded as having excellent potential for printable solar cells, was studied and patented as a good light-emitting device material many years ago [21,22]. Because, in terms of physical principles, a light-emitting device is the reverse of a solar cell, it is quite natural to consider light-emitting materials to discover materials that are good for use in solar cells. Therefore, it appears that the discovery of halogen perovskites for solar cells was made by incorporating halogen perovskites as light-emitting materials in solar cell applications, based on the common ground of physics in photo-electron energy conversion. The other example is catalysts for fuel cells that do not contain metals, such as Pt, but contain only carbon and nitrogen (the so-called carbon alloy catalyst). Before the discovery of this carbon alloy catalyst, no one seems to have searched for such non-metallic catalysts for use in fuel cells; here the use of Pt is usual, but efforts to reduce the amount of Pt are the main stream of research developments. However, the catalytic activity of carbon in the organic synthesis field has long been known: some types of carbon were reported to work as a catalyst for oxidation of oxalic acid [23] and carbon containing nitrogen worked even better with this [24] and other cases. Therefore, it appears that the carbon alloy catalyst was discovered by combining knowledge on catalytic activity of carbon or nitrogen-containing carbon for oxidation with fuel cell catalysis application.

3. Characteristic Features of the Tool

When users require a „good‟ material, they mostly use those already developed, and attempt to improve the properties, such as strength, of those already in use. However, users do not need materials with better properties, but they need ones with specific properties that are suitable for their intended purpose (for what they want to achieve). This tool aims to realize "wants" of users without using customs or conventions. The focus on users‟ "wants", not "needs" should be emphasized. Once "wants" become clear, we can list ways to achieve them according to scientific principles. The flowchart for drawing design principles with the tool is shown in figure 5. As mentioned above, using alternatives to customs or conventions (supplier side viewpoint) is an important preparatory step in drawing design principles (step 0 in the figure). Via this step, one is able to discover "wants" of the users (step 1). The next step (step 2) is to describe conditions that achieve the "wants" from the point of view of scientific principles. Here, only the essential conditions according to scientific principles should be considered, without bothering with technical or other possibilities. The methods that satisfy the conditions from the principles are listed in the next step (step 3). Again, it is not necessary to consider whether the method is realistic in practice or not. Up to this step, the process is similar to the brain storming method and involves relating and combining different kinds of materials quantities. After listing all possible methods, each should be examined, one-by-one, using a knowledge database, such as various mathematical relationships among physical quantities and materials databases (step 4). From step 4, materials design principles are obtained and the selection of materials to be explored is carried out (step 5). An example of the flow for the case of 2.3 (substrate suitable for the growth of atomically flat epitaxial alumina film) is described below. In this case, "wants" is "substrate suitable for the growth of atomically flat epitaxial alumina film". A textbook on film growth tells us that for flat growth FM growth is required among three major models, SK, FM and VW, of which difference comes from differences in interfacial energy and strain energy. It is known that symmetry and lattice matching are important in epitaxial growth. Getting those knowledge coming from scientific principles is the process for step 2. Then, concluding the use of Al-containing alloy having the surface with six-fold symmetry, which have a lattice constant commensurate to alumina is the process for step 3. During this step, other possibilities have been excluded by considering quantities such as adsorption energy, interfacial energy and surface energy in databases or handbooks. Finally, by utilizing database on phase diagram to check solubility of aluminium and on crystal structure for symmetry and lattice matching, a suitable substrate is found (step 4 and 5).

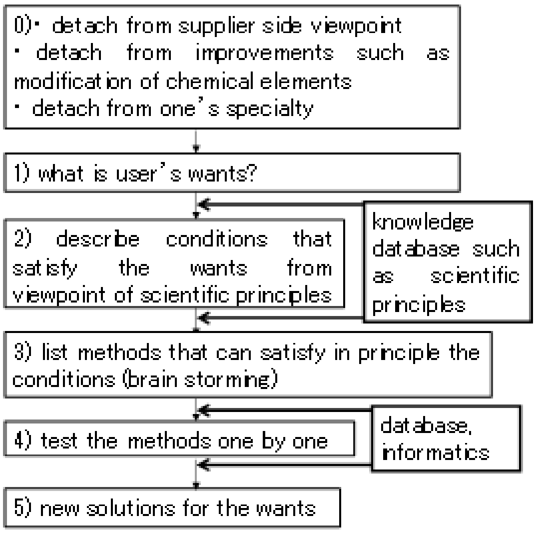


Figure 5: The flowchart for drawing design principles with the presented tool.

Figure 6 shows the concept of the selection, combination, and multidisciplinary editing of the contents. The groups A-D are already-established categories, where material data and knowledge are contents, a, b, c, d, d‟, etc. By combining contents from points X and Y, contents a and d now belong to X, whereas b, c, and d‟ belong to Y. A new relationship is then found between X and Y, which gives a new meaning to the contents a, b, c, d and d‟. Applying, for example, the figure to the example in section 2.1 (work function tuning), A, C, D are device physics, metallurgy, and surface physics, respectively (here, we used three different categories, and nothing corresponding to B). X and Y are the work function and composition, respectively. The method, illustrated in figures 5 and 6, is very different from the so-called materials informatics, that at present handle vast amounts of information with statistics. Instead, scientific principles are treated as a part of information in the proposed tool. For example, the case of section 2.1 (work function tuning) uses information that SBH is, ideally, linearly dependent on work function of the electrode, that composition dependence of work function in binary systems follows a certain pattern, according to the types of phase diagram of the binary systems, etc. Relating work function with phase diagram was new at the time in the device materials field. With this property, the author was successful in relating work function with Vickers hardness in a specific group of materials [25]. Likewise, it should be possible to make connections among different physical or chemical properties based on scientific principles. An example of such connections is illustrated in figure 7. A huge network of connections must be made if all the current knowledge on materials science is taken into account. Creating such a network of connections and developing computational techniques to find quantities and relationships that are connected to a target property in the network would enable efficient progress of step 2 and 3 in figure 5. A test software to store connections such as the example and to find a network path leading to a target property has already been developed by the author.

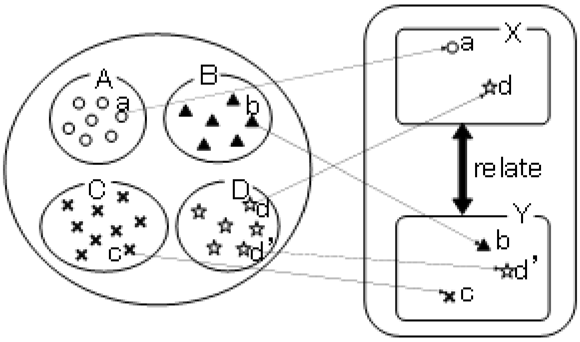


Figure 6: Schematics of the concept of the selection, combination and multidisciplinary editing of the contents. The groups A-D are already-established categories, where material data and knowledge are contents, a, b, c, d, d‟, etc. By combining contents from viewpoints X and Y, contents a and d now belong to X, whereas b, c and d‟ belong to Y. A new relationship is then found between X and Y, giving a new meaning to the contents a, b, c, d and d‟.

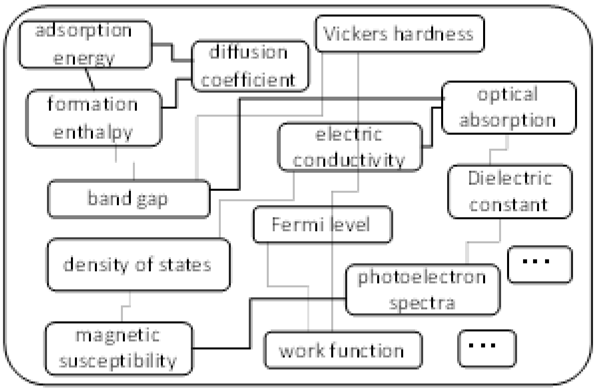


Figure 7: Schematic of connections among different physical or chemical properties, based on scientific principles.

4. Relationship between the tool and other data-related techniques

Using the proposed tool, design principles are obtained and subsequently, various databases are searched with the aid of informatics to suggest concrete materials that match these design principles. High throughput synthesis/analysis/ theoretical calculations need to be applied to optimize suggested materials for practical use. The relationships between database, informatics, the presented tool (materials curation), and high-throughput techniques are shown in figure 8.

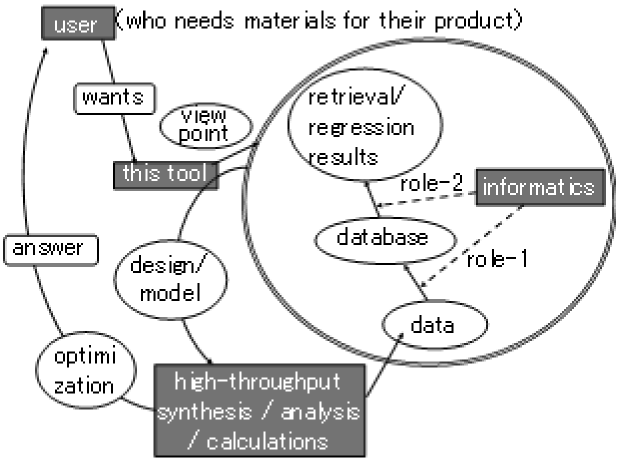


Figure 8: Schematic of the relationship between database, informatics, the presented tool (materials curation), and high-throughput techniques.

At present, parts of the scheme are incomplete. Much data on properties, such as electronic conductivity, elastic modulus, and optical absorbance, are missing on already-discovered materials whose crystal structures have been identified. For the efficient progress of step 4 and 5 in figure 5, data are highly desired to be electronically retrievable. However, often, the required information in databases cannot be retrieved although the data exist. For example, retrieval of materials with electric conductivity greater than 10^6 [S/m] is impossible in handbooks such as CRC Handbook [26] (even in electronic version) or even in the web-retrievable free material database MatNavi [27]. This is a problem associated with retrieved items in databases using informatics (role-1 in figure 8). In addition, even when retrieval from reported properties is possible, it may be difficult making a correlation diagram between different properties, such as electric conductivity and thermal conductivity in a free material property database MatWeb [28]. The role-2 in figure 8 is responsible for this type of problems. The tool presented here is, of course, only an initial proposal, and a long way from being complete. Further development of several aspects of high-throughput techniques is still required. There are three major techniques in high-throughput: synthesis, analysis, and computer simulations. With synthesis, combinatorial methods, especially thin film deposition and chemical synthesis, have been developed for optimizing materials composition. However, combinatorial synthesis of bulk solid materials seems to be still on its way. There seem to be almost no high-throughput techniques for synthesis process optimization, such as temperature of a process and flow rate of gases. High-throughput analysis of combinatorial materials libraries using imaging techniques has developed significantly. However, each different type of analysis, such as crystal structure by X-ray diffraction (XRD) and refractive index by optical spectroscopy, has to be done separately. It is necessary to have one-stop type analyses, where many different basic properties of a specimen are analysed automatically once the specimen is introduced in a multiple-analysis system; these can be carried out, by integrating leading-edge downsizing instrumentation technologies, such as portable XRD analysers [29] and mini-spectrometers [30]. With computer simulations, several efforts have just started to appear, such as high-throughput first-principle calculations with density functional theory, molecular dynamics simulations, and multiscale simulation. Development of all the above techniques, together with this proposed materials design tool is essential for accelerating material development. It should be noted that although this materials design tool can suggest a new type of a candidate material, apart from those that have already been studied in the field, it does not determine the one with the best performance.

5. Summary

A tool is proposed to draw materials design principles and search for materials systematically with a comprehensive and panoramic view by using existing materials information through a cross-sectoral and multidisciplinary approach. Examples of material search with the tool are demonstrated, and its characteristic features are explained. The tool is called “materials curation”, following the concept of “content curation” in the information business field, with its typical features of “combining things in a multidisciplinary approach”.

Although the task of combination in the examples was manually done, it can be done using an appropriate computer program, because the combination is completely based on scientific principles. In fact, finding a connection between two target properties in a diagram such as Fig. 7 is possible using a computational technique in the field of graph theory [31]. One of the major aims of this article is to call upon like-minded members to construct a materials design tool to cover the full range of possibilities. The range in which the author is able to combine information is limited to some extent. In order to construct a computer-aided curation system, cooperation from scientists from a wide range of fields is essential.

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[4] Wikipedia, “Content curation is the process of collecting, organizing, and displaying information relevant to a particular topic or area of interest. Services or people that implement content curation are called curators. Curation services can be used by businesses as well as end users.

Content curation is not a new phenomenon. Museums and galleries have curators to select items for collection and display. There are also curators in the world of media, for instance RJs tasked with selecting songs to be played over the air. Content curation can be carried out either manually or automatically. The former is done by specially designated curators. The latter is done using one or more of the following: collaborative filtering, semantic analysis, or social rating." Available: https://en.wikipedia.org/wiki/Content_curation. [Accessed: Sept. 22, 2015].

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