Solving the Mysteries of the Solid Elements (From the Origin of Elements to Machine Parts)

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PREFACE

Most of the elements on the periodic table are solid elements. The solid elements have various properties, respectively. Frequently, the properties of the elements are listed at the end of books on materials science or metallurgy. But they are only shown as a matter of form. The reasons why each element has such properties are not shown.

The periodic table is the only one which shows the relative relationship to each other among elements. But it is a pity that it shows only the similarities of chemical properties in the same group.

It shows very little about the atomic radius, crystal structure, melting point, Young's modulus, thermal conductivity and so on.

Furthermore, the similarity of the chemical properties is only valid at the elements in the 1st, 2nd, 18th group – alkali metals, alkaline earth metals and halogen.

For example, the elements in the 14th group – C, Si, Ge, Sn, and Pb – show very different chemical properties. Shortly, the periodic table shows very little about the solid elements.

Taking these situations into consideration, a new representation of the elements is desired.

This author has set two assumptions.

In general, the main characteristics of the solid elements are their crystal structures and their possession of free electrons.

Among many physical properties, lattice strength, as represented by Young's modulus, and free electron mobility, as represented by thermal conductivity, were therefore selected for their characterization.

Consequently, a diagram was made with the thermal conductivity on the abscissa and the Young's modulus on the ordinate, and each element was plotted on the diagram. This diagram was referred to as the **"thermal conductivity-Young's modulus" (TC-YM) diagram.**

On the other hand, there are many mysteries in the solid elements. For instance, most of the solid elements adopt various crystal structures. But it is not known whether there is a rule which determines the crystal structures of the elements. There are many other mysteries left unsolved in the solid elements.

Here, the results of the studies having applied the TC-YM diagram to these mysteries will be shown.

This book is full of many original figures which mankind has never seen about the basic properties of elements.

1. PREPARATION OF THE KEY FOR SOLVING THE MYSTERIES OF THE SOLID ELEMENTS

Looking at books on the solid elements, the various properties of the elements such as atomic number, atomic mass, density, atomic volume, melting point, boiling point, specific heat, fusion heat, linear expansion coefficient, thermal conductivity, electrical resistance, Young's modulus, crystal structures, lattice constant, etc., are listed in a table. They are shown equally.

In the properties of the elements, there are **base quantities** and **derived quantities**. The density of the element is clearly a derived quantity, because it is determined by the atomic mass, atomic radius and the crystal structure. The base quantity is a quantity which cannot be determined by other quantities. But, in practice, it is difficult to judge which are the base quantities and derived quantities in the material properties of the elements. For instance, the melting temperature and the Young's modulus are considered to be base quantities and independent of each other. But it can be speculated that the melting temperatures of elements are determined by the Young's modulus. Fig. 1-1 shows the relationship between the melting temperatures of elements and the Young's moduli of elements.

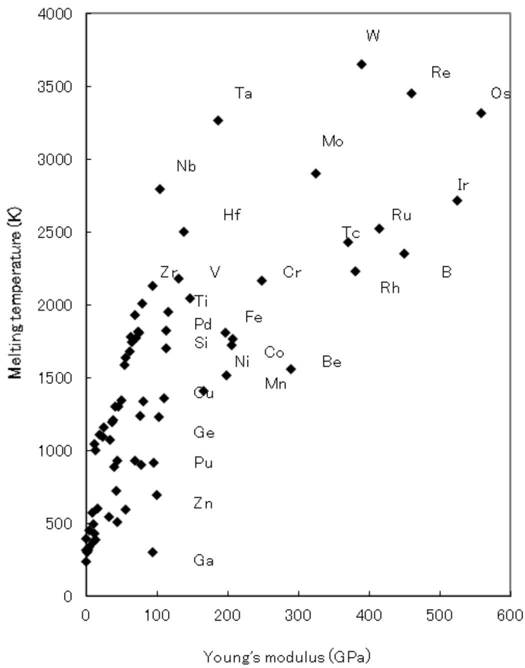

Fig. 1-1 – Melting temperatures of elements as a parameter of Young's modulus

A rough tendency that the melting temperature is proportional to the Young's modulus is recognized. But, W having the highest melting temperature does not have the largest Young's modulus. In addition, the elements possessing a similar Young's modulus of about 100 GPa – Ga, Zn, Pu, Ge, Cu, Si, Pd, Ti, and Zr – show a very large range of melting temperature.

Therefore, it can be speculated that it is impossible to represent one property with one base quantity such as Young's modulus, and at least one more base quantity would be necessary. Two base quantities and one property form three-dimensional space, and can be displayed on the plane, if the property is shown by layers. More than two base quantities cannot be displayed on a plane. Therefore, two base quantities were sought in this study.

As a result, the Young’s modulus and thermal conductivity were selected as two base quantities.

The reason why the elements possessing a similar Young’s modulus of about 100 GPa – Ga, Zn, Pu, Ge, Cu, Si, Ti, and Zr – show a very wide range of melting temperatures will be shown in Chapter 4.

1.1 Introduction of the TC-YM diagram

This author has introduced a new diagram to explain the behaviors of elements. In general, the main characteristics of the metallic elements are metallic bonding of atoms and the existence of free electrons.

Among many physical properties, the Young's modulus was selected as a representative index for the strength of the lattice; thermal conductivity was selected as a representative index for the characteristics of free electrons.

Young’s modulus is a gradient of the stress-strain curve in the region of elasticity in the tensile test, as shown in Fig. 1-2.

The Young’s modulus relates also to the atomic structures of the materials. Fig. 1-3 shows the interatomic force between two atoms. [1]

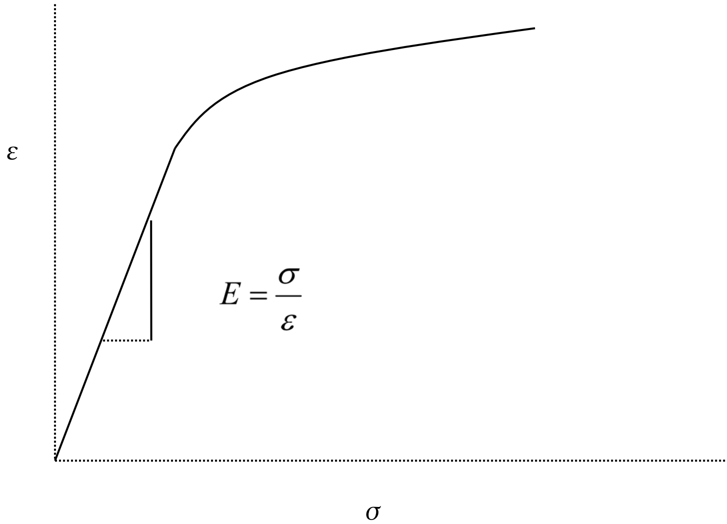

Fig. 1-2 – Stress-strain curve of a tensile specimen and its Young's modulus

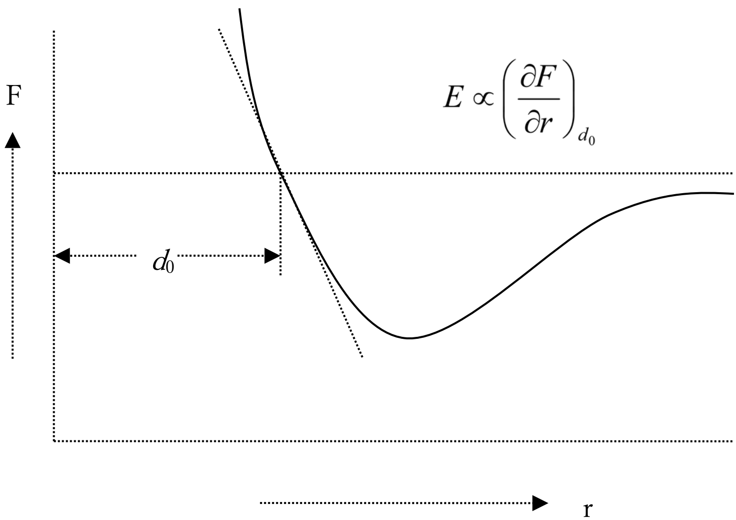

Fig. 1-3 – Interatomic force versus interatomic distance

The repulsive force acts within d_0, and the attractive force acts outside d_0. The gradient of the tangent at d_0 is proportional to the Young's modulus. Therefore, the Young's modulus is a substantial factor which represents the state of atoms.

Consequently, a diagram was made with the thermal conductivity on the abscissa and the Young's modulus on the ordinate, and each element was plotted on the diagram. This diagram will be referred to as the "thermal conductivity-Young's modulus" (TC-YM) diagram.

Young's modulus is generally thought to be an engineering factor, but it is a physically fundamental factor: The Young's modulus is proportional to the gradient of the tangent of the curve of the Condon-Morse force between atoms at an equivalent atomic distance [1] i.e., proportional to the second-order differential of the binding potential between two atoms at equivalent atomic distance. [2] Young's modulus is therefore a good index to represent the binding state of atoms.

Thermal conductivity can be considered to be related to the mobility of free electrons in atoms. This is also a physically fundamental factor.

A diagram with thermal conductivity on the abscissa and Young's modulus on the ordinate (TC–YM diagram) can therefore reflect the essential properties of atoms of the metallic and semi-metallic elements.

The thermal conductivity is said to come from both the free electron transfer and the lattice vibration. [3] The ratio of the thermal conductivity to the electrical conductivity is constant at room temperature and is called the Wiedemann-Franz law. [4] Fig. 1-4 shows the relationship of solid elements between the thermal conductivity and the electrical conductivity.

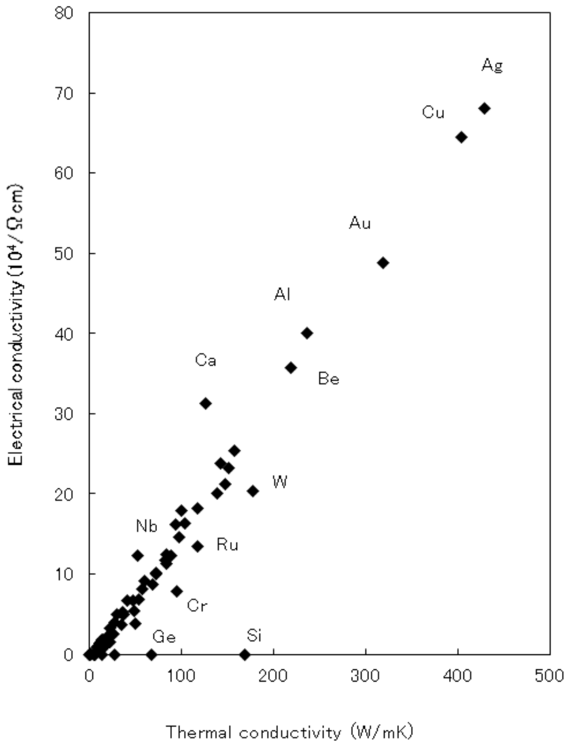

Fig. 1-4 – Relationship in the elements between the thermal conductivity and the electrical conductivity

Except for the semi-conductor elements Ge and Si, the thermal conductivity is proportional to the electrical conductivity in all solid elements. Fig. 1-4 shows that the thermal conductivity is covered by the free electrons in the solid elements.

Then, how about the contribution of the lattice vibration to the thermal conductivity?

To examine this, the result of taking the correlation between the thermal conductivity and the Young's modulus as the factor of lattice vibration is this TC-YM diagram. The result is shown in Fig. 1-5. [5]

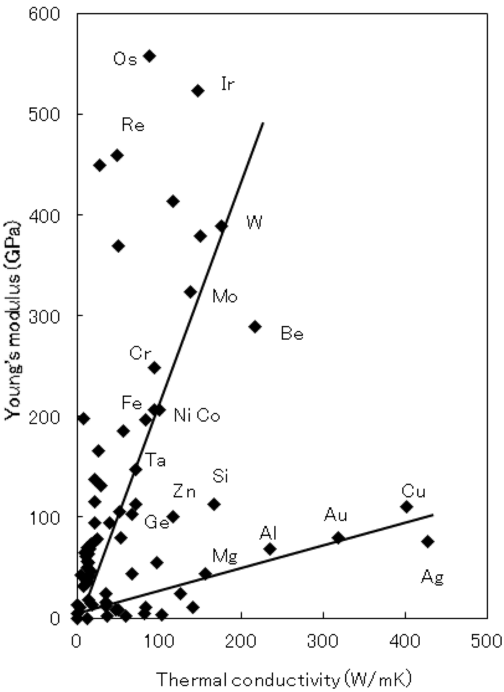

Fig. 1-5 – Relationship in the elements between the thermal conductivity and the Young's modulus

At first glance at this figure, this author felt that there were some patterns hidden in it. **It was felt as if it were a starry sky of elements viewed from**

the window of a house. Some constellations can be seen. What does each constellation mean? This is the subject of this book.

In this case, the semiconductor elements – Ge and Si – are contained in the figure. Moreover, Ge and Si show behaviors similar to the nearby elements such as the alloying elements, as shown subsequently. Further, the half metallic elements, such as As, Se, Te, and I, show the intrinsic characteristics according to their positions in the TC-YM diagram. In this way, the TC-YM diagram shows the characteristics of most solid elements, including metallic, semiconductor and half metallic elements.

As shown in Fig. 1-5, there is an element group of Mg, Al, Au, and Cu in which the thermal conductivity abruptly increases with only a slight increase of the Young's modulus, and there is an element group of Ta, Fe, Ni, Co, Cr, Mo, and W in which the thermal conductivity increases modestly with the increase of the Young's modulus. However, there are many additional elements that are randomly distributed in the TC-YM diagram.

As shown in Fig. 1-4, the thermal conductivity is covered by the transfer of the free electrons; therefore, the Young's modulus is freed from the contribution to the thermal conductivity, and is able to take free values, enabling the elements of high thermal conductivity and low Young's modulus and those of low thermal conductivity and high Young's modulus.

To confirm the validity of this diagram, firstly, it was tested if the diagram could show the crystal structures of elements significantly.

Fig. 1-6 shows the distribution of the crystal structures of various elements in a TC-YM diagram.

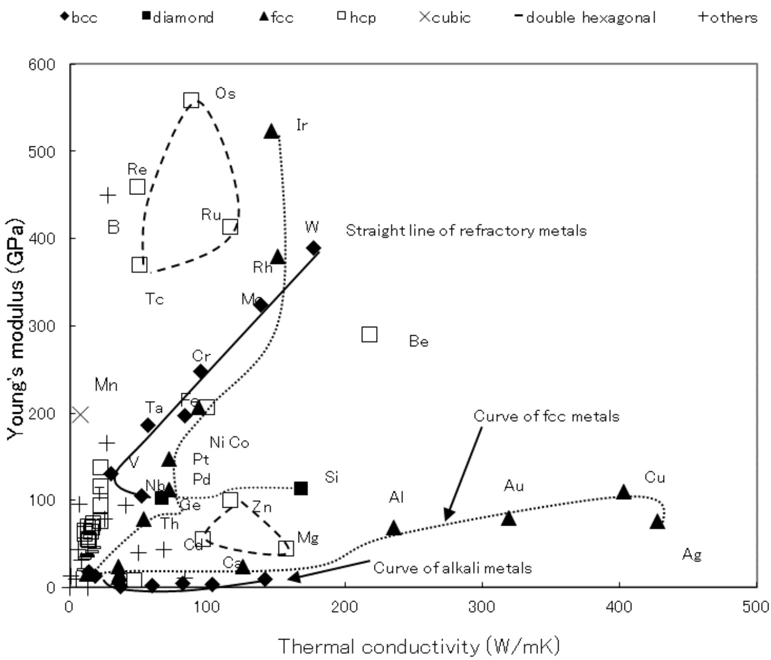

Fig. 1-6 – Crystal structures of elements shown on the TC-YM diagram

The crystal structures are classified as body-centered-cubic (bcc), face-centered-cubic (fcc), hexagonal-close-packed (hcp), diamond structured, and “others” for miscellaneous structures. [6] The most remarkable feature of Fig. 1-6 is that the bcc-structured elements mostly lie on a straight line, connecting V, Ta, Cr, Mo, and W, which can be called *the straight line of refractory metals*. At the moment this author looked at this, he was convinced of the validity of the diagram. Iron is located near this line.

Additionally, elements with fcc structures lie on a clear curve, which can be called *the curve of fcc metals*. It took some time for this author to find the curve of fcc metals. When he did, he was convinced further of the validity of the diagram.

In contrast, bcc-structured alkali metals lie on a curve near the abscissa (*the curve of alkali metals*). Elements with hcp and other structures are distributed elsewhere. Lanthanides gather tightly in the low Young's modulus and low thermal conductivity region. In the periodic table, the lanthanides are shown outside the table, and the relationships with other elements are lost.

The TC-YM diagram, therefore, shows clear patterns with respect to the crystal structures of elements. Other elemental properties, such as atomic radius, melting temperature, thermal expansion, boiling point, heat of fusion, vapor pressure, heat capacity, electronegativity, and ionization energy, also show clear patterns in TC-YM diagrams.

The details of the crystal structures will be discussed in Chapter 2.

1.2 Distribution of elements on the TC-YM diagram per period in the periodic table

There was an examination of the kind of relationship that exists between the TC-YM diagram and the periodic table.

Fig. 1-7 shows the distribution of elements of the 2nd, 3rd, and 4th periods on the TC-YM diagram, respectively. The elements of the same period draw a cycle. It starts from the bottom of the diagram, and goes up toward the high thermal conductivity and high Young's modulus region. And then, it decreases the thermal conductivity and finally decreases the Young's modulus and goes down to the origin of the diagram. With the increasing period number, the form of the cycle becomes complicated.

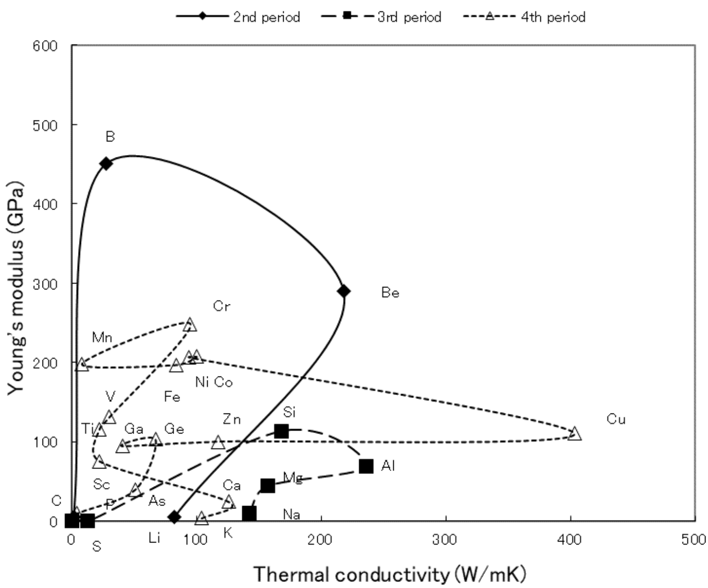

Fig. 1-7 – Distribution of elements of the 2nd, 3rd, and 4th periods on the TC-YM diagram

Fig. 1-8 shows the distribution of elements of the 5th, 6th, and 7th periods on the TC-YM diagram, respectively. The elements of each period draw a complicated cycle. It starts from the bottom, goes up with decreasing conductivity, and then goes up further with increasing conductivity. After reaching the peak, it goes down with decreasing conductivity. And then, it increases the conductivity abruptly. After that, it again decreases the conductivity abruptly and ends near the origin.

Young's modulus of Tc: Tc is an unstable and radioactive element. It is said that Tc is the first man-made element. Data on its Young's modulus are missing. As shown in Fig. 1-8, the forms of the cycles of the 5th period and the 6th period are similar to each other. The thermal conductivity of Tc is reported to be 50.6 W/mK. Therefore, the Young's modus of Tc can be speculated to be around 370 GPa from the similarity of the forms of the cycles. The speculated position of Tc is plotted on Fig. 1-8. This position of Tc on the TC-YM diagram will be proved to be valid in other properties of Tc.

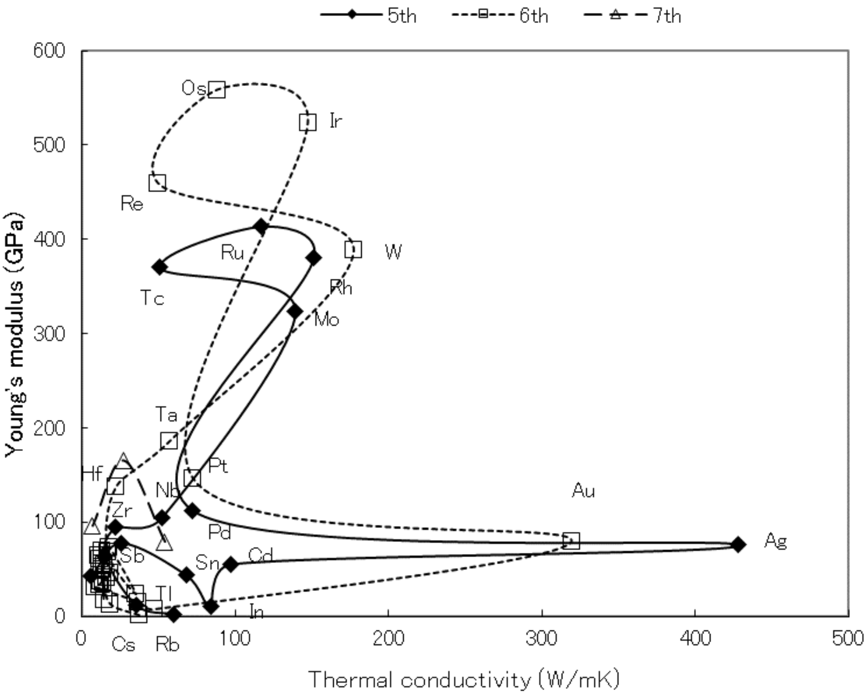

Fig. 1-8 – Distribution of elements of the 5th, 6th, and 7th periods on the TC-YM diagram

1.3 Distribution of elements on the TC-YM diagram per group in the periodic table

One of the greatest characteristics of the periodic table is that elements of the same group have similar properties, especially in chemical properties. But elements of group 13 – B, Al, Ga, In, and Tl – and those of group 14 – C, Si, Ge, Sn, and Pb – cannot be said to have similar properties.

Fig. 1-9 shows the distribution of elements on the TC-YM diagram per group (from group 1 to group 10). The elements of the same group show each line.

Fig. 1-10 shows the distribution of elements on the TC-YM diagram per group (from group 11 to group 16).

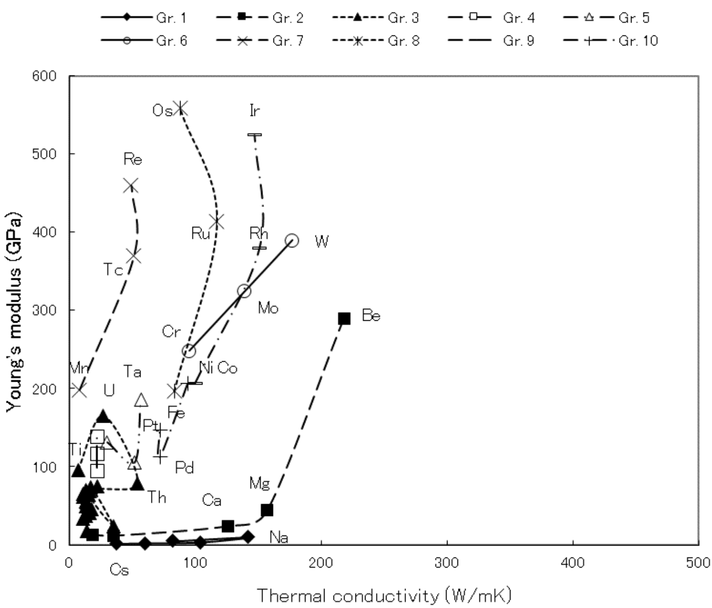

Fig. 1-9 – Distribution of elements on the TC-YM diagram per group (from group 1 to group 10)

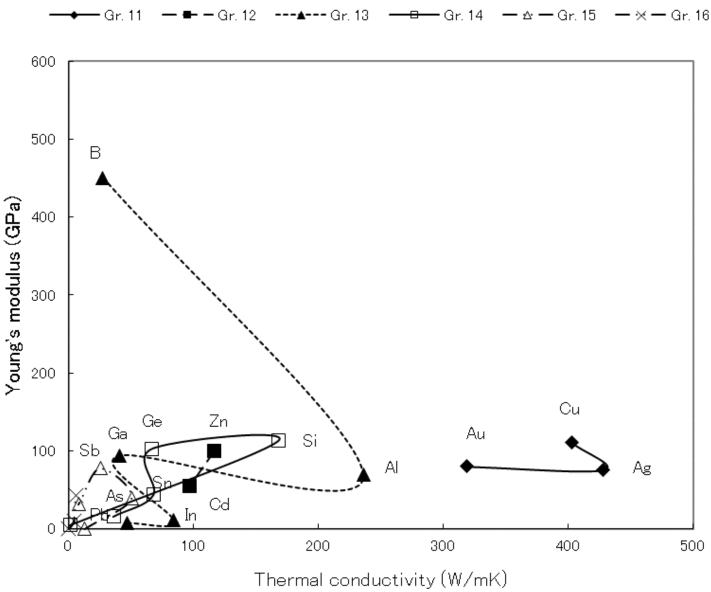

Fig. 1-10 – Distribution of elements on the TC-YM diagram per group (from group 11 to group 16)

The elements of group 1 (alkali metals) commonly show very low Young's modulus. Only the thermal conductivity varies with different inner electron shells.

The elements in group 2 (alkaline earth metals) commonly show also very low Young's modulus except for Be. Only the thermal conductivity varies with varying inner electron shell.

The trend changes in group 3.

The elements of group 3 – Sc, Y, lanthanides and actinides – commonly show very low thermal conductivity except Th, U and Pu. Only the Young's modulus varies with varying inner electron shell in the low Young's modulus range.

The elements of group 4 – Ti, Zr and Hf – also commonly show very low thermal conductivity. Only the Young's modulus varies with varying inner electron shell.

The trend changes in group 5.

The elements of group 5 – V, Nb and Ta – show the Young's modulus proportional to the thermal conductivity except for Nb. Both the Young's modulus and the thermal conductivity vary with varying inner electron shell.

The elements of group 6 – Cr, Mo and W – also show the Young's modulus proportional to the thermal conductivity. Both the Young's modulus and the thermal conductivity vary with varying inner electron shell. With increasing inner electron shell, both the Young's modulus and the thermal conductivity increase.

The trend changes in group 7.

The elements of group 7 – Mn, Tc and Re – commonly show low thermal conductivity. The Young's modulus varies with varying inner electron shell.

The elements of group 8 – Fe, Re and Os – commonly show a little larger thermal conductivity. The Young's modulus varies with varying inner electron shell. Os has the largest Young's modulus among elements.

The elements of group 9 – Co, Rh and Ir – commonly show a little larger thermal conductivity. The Young's modulus varies with inner electron shell.

The elements of group 10 – Ni, Pd and Pt – commonly show medium thermal conductivity. The Young's modulus varies with varying inner electron shell, but these values are smaller than in the former groups.

The trend changes in group 11.

The elements in group 11 – Cu, Ag and Au – commonly show low Young's modulus. The thermal conductivity varies with varying inner electron shell. The values of the thermal conductivity commonly are large.

The elements in group 12 – Zn, Cd and Hg – commonly show low Young's modulus except for Hg. The thermal conductivity varies with varying inner electron shell.

The elements in group 13 – B, Al, Ga, In and Tl – commonly show low Young's modulus, except for B. The thermal conductivity varies with varying inner electron shell.

The elements in group 14 – C, Si, Ge, Sn and Pb – commonly show low Young's modulus. The thermal conductivity varies with varying inner electron shell.

The elements in group 15 – P, As, Sb and Bi – commonly show very low Young's modulus. The thermal conductivity varies with varying inner electron shell. But the varying range is small.

The elements in group 16 – S, Se and Te – commonly show very small Young's modulus. The thermal conductivity doesn't vary any more, and commonly adopts very small values.

In conclusion, the following can be said:

The binding force between atoms represented by the Young's modulus and the mobility of free electrons represented by the thermal conductivity is roughly decided by the electron configuration in the outer shell, and thereafter, it is decided by the structure of the inner shell.

It has been said that the properties of elements are decided solely by the electron configuration in the outer shell. This assumption must be corrected.

1.4 Distribution of the lanthanides on the TC-YM diagram

As shown in Fig. 1-8, the lanthanides of the 6th period are crowded in the region of low thermal conductivity and low Young's modulus. Fig. 1-11 shows the distribution of the lanthanides at the range of low thermal conductivity and low Young's modulus of the TC-YM diagram. The 6th period starts from Cs on the bottom. It goes up with decreasing thermal conductivity through Ba to La. The lanthanides begin from La. It goes up in a winding way. It reaches finally Lu, and Lu connects to Hf. But on the way, anomalies happen, namely, Eu and Yb drop abruptly. This will be discussed in Chapter 6.

The lanthanides have been displayed separately from the main elements in the periodic table. But in the TC-YM diagram, they are displayed together with other elements. Their locations are variable on the diagram, and their properties are variable according to their locations.

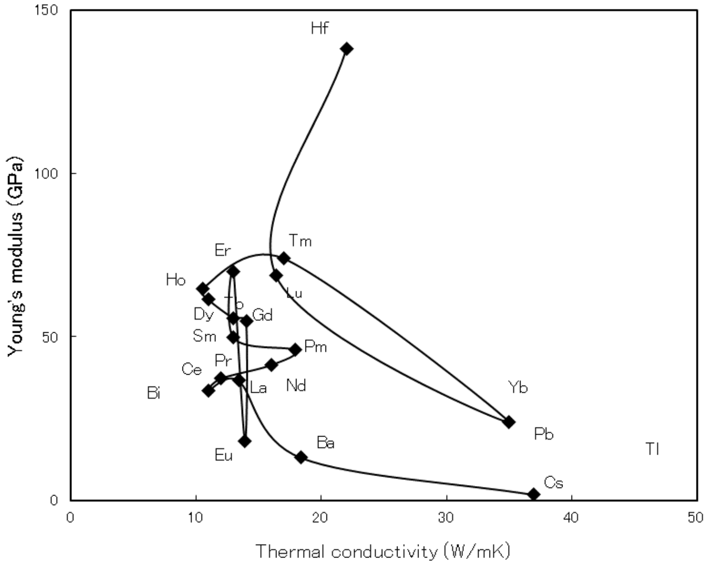

Fig. 1-11 - Distribution of the lanthanides on the TC-YM diagram

1.5 Young's modulus and thermal conductivity of elements on the periodic table

To be sure, the distributions of both the Young's modulus and thermal conductivity of elements on the periodic table are shown in Figs. 1-12 and 1-13, respectively.

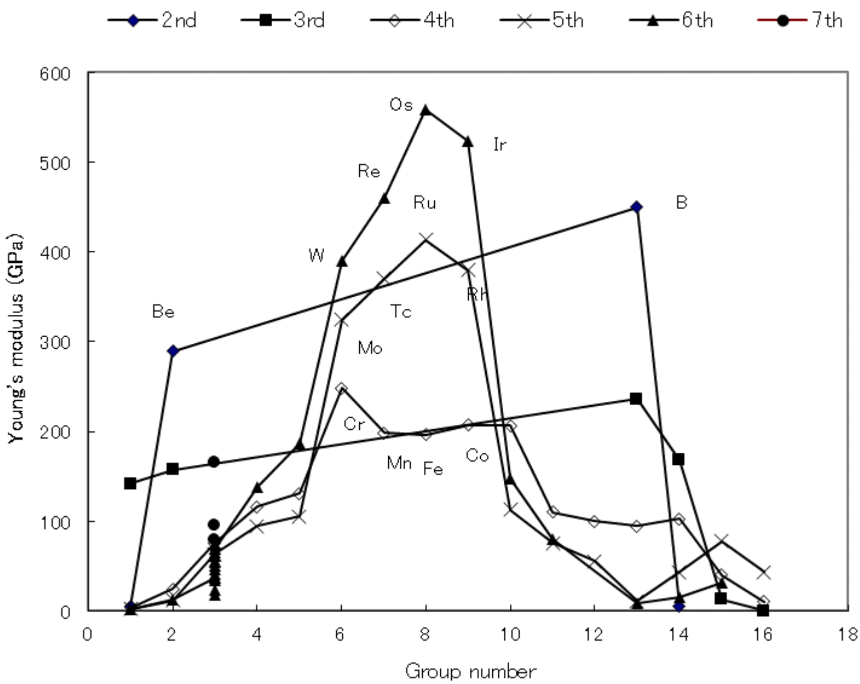

Fig. 1-12 – Young's moduli of elements as a parameter of the group number in the periodic table

The Young's moduli of elements show, as a whole, mountain-like patterns with the peaks at group 8. These patterns are similar to those of the melting temperatures of elements shown in Figure 4.1. But the positions of their peaks are different to each other. Melting temperatures adopt their peaks at group 6, but Young's moduli adopt their peaks at group 8. Therefore, there is no linear relationship between melting temperatures and Young's moduli of elements, as shown in Fig. 1-1.

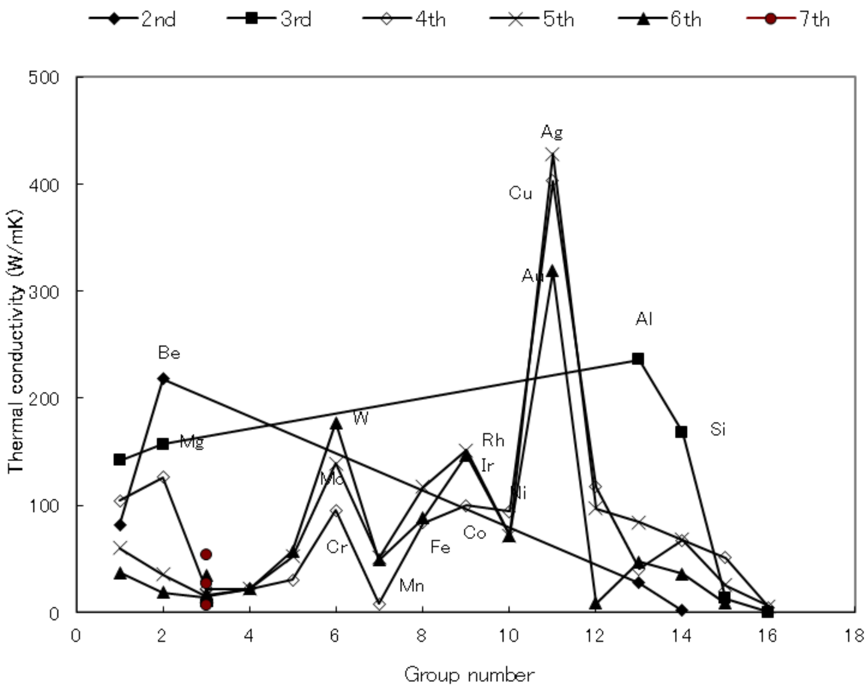

Fig. 1-13 Values of the thermal conductivity of elements as a parameter of the group number in the periodic table

In contrast to the Young's modulus, the thermal conductivity of elements shows complicated patterns on the periodic table, as shown in Fig. 1.13. It goes up and down with increasing atomic number. It is impossible to read a tendency from this figure.

Fig. 1-14 shows the variation of the Young's modulus of the lanthanides as a parameter of the atomic number, and Fig. 1-15 shows the variation of the thermal conductivity of the lanthanides as a parameter of the atomic number, respectively.

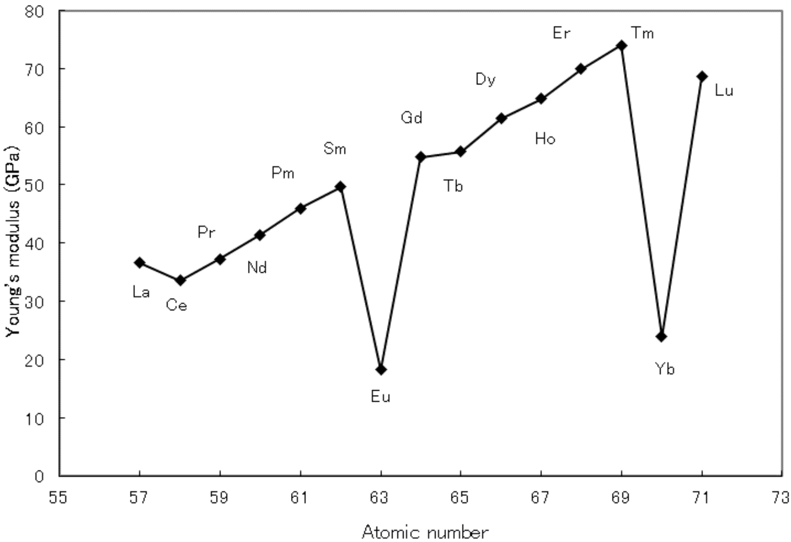

Fig. 1-14 – Young's moduli of the lanthanides as a parameter of the atomic number in the periodic table

The Young's modulus increases with increasing atomic number. But it drops abruptly at Eu and Yb.

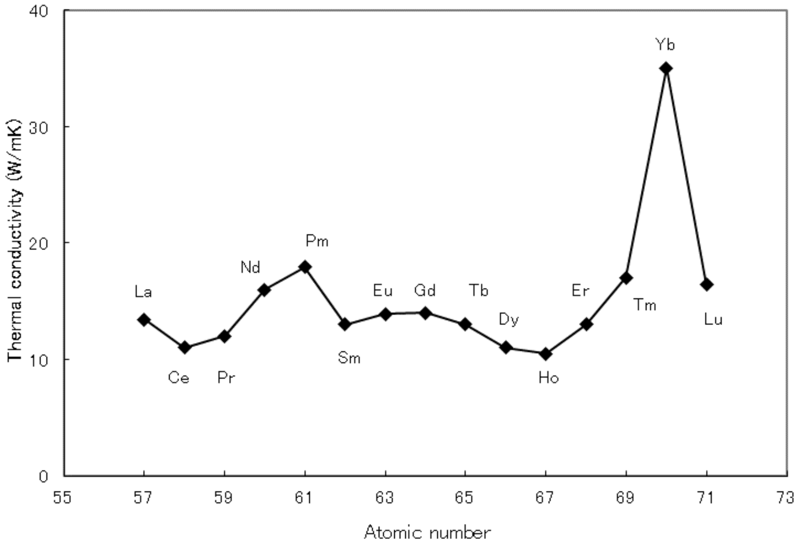

Fig. 1.15 – Values of thermal conductivity of the lanthanides as a parameter of the atomic number in the periodic table

The thermal conductivity of the lanthanides is constant with the atomic number. But it adopts a large value at Yb.

These anomalies can be explained on the TC-YM diagram, as discussed in Chapter 6.

Fig. 1-16 shows the variation of the Young's modulus of the actinides as a parameter of the atomic number, and Fig. 1-17 shows the variation of the thermal conductivity of the actinides as a parameter of the atomic number, respectively.

Data are scarce regarding the actinides. The tendency cannot be read from these figures. Details will be discussed in Chapter 7.