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Correlation of the Fermi Energy and Others to the Electron Charge-Discharge Characteristics of Atoms

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***Abstract* —**

As the examples of electron charge-discharge characteristics of elements, the electrode potential, electronegativity, ionization energy and electron affinity were examined. They are plotted on the TC-YM diagram developed by the author recently. They showed the clear patterns on the diagram, corresponding to each characteristic. It was recognized that there are clear differences between these characteristics.

Next, their correlations to the periodicity in the periodic table, atomic radius, and Fermi energy were studied. But they showed abrupt changes or vague tendencies.

Consequently, it is concluded that the TC-YM diagram is the best way to represent the electron charge-discharge characteristics of elements.

Keywords – *Electrode potential, Electronegativity, Ionization energy, Electron affinity, Fermi energy*

I. INTRODUCTION

There are several quantities which describe the electron charge-discharge characteristics of atoms. Specifically, they are the electrode potential, electronegatiity, ionization energy, and electron affinity. They are subtly different to each other in the definitions and values. On the other hand, there is a quantity which is called the Fermi energy, which means the maximum energy of electron in the conduction band of the metallic elements.

The author introduced TC-YM diagram which complements the periodic table and interpret the characteristics of elements. The author has already clarified the rule of crystal structures of elements [1], the solubility of elements in metals [1], the rule of melting temperatures of elements [2], the rule of the abundance of elements in the universe [3], the mechanism of hardenability of steels [4], and the rule of crystal structures and properties of the lanthanides[5], the mechanism of the neutron absorption of Zr [6], and the crystal structures of elements after the allotropic transformations [7].

Here, using the TC-YM diagram, several electron charge-discharge characteristics of atoms and the Fermi energy of elements were studied.

II. ELECTRON CHARGE-DISCHARGE CHARACTERISTICS OF ATOMS

The periodicity of the ionization energy has been frequently referred to as the good example of the periodicity of the atomic structure. Figure 1 shows the variation of the ionization energy of the solid elements in order of atomic number. The alkali metals show small ionization energies. The ionization energy increases as the atomic number increases within s given period. This has been considered to be evidence that verifies the validity of the periodic table. But, the situation of the increase is not simple, as shown in Figure 1. There must be some reasons hidden in it.

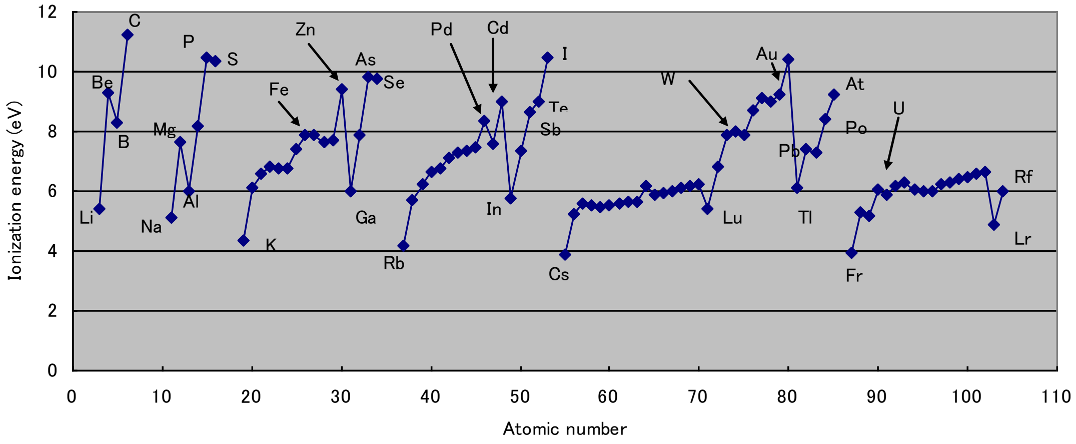

Figure 1: Ionization energies of elements and atomic number

To clarify the electron charge-discharge characteristics of atoms, the electrode potential, electronegativity, ionization energy, and electron affinity were studied.

A. Electrode potential

The electrode potential refers to the ease with which the electrons are discharged from the metallic elements in the aqueous solution [8, 9]. The higher the electrode potential is, the harder the discharge of electrons from the metallic element is.

The values of the standard electrode potential of elements are plotted on the TC-YM diagram and shown in Figure 2. The figures in the legend show the range of the electrode potential in units of V.

The elements of the smallest thermal conductivities show small electrode potential. With increasing thermal conductivity, the electrode potential of elements increases up to Au, Cu , and Ag. But on the way, the electrode potential of elements lowers at W, Be, Si, and Al.

With increasing Young’s modulus, the electrode potential of elements increases.

The total pattern is different from the patterns obtained so far in other properties. The elements Ir, Au, and Pt are the poles of the electrode potential on the TC-YM diagram. The elements in their neighborhood also show similar characteristics to them.

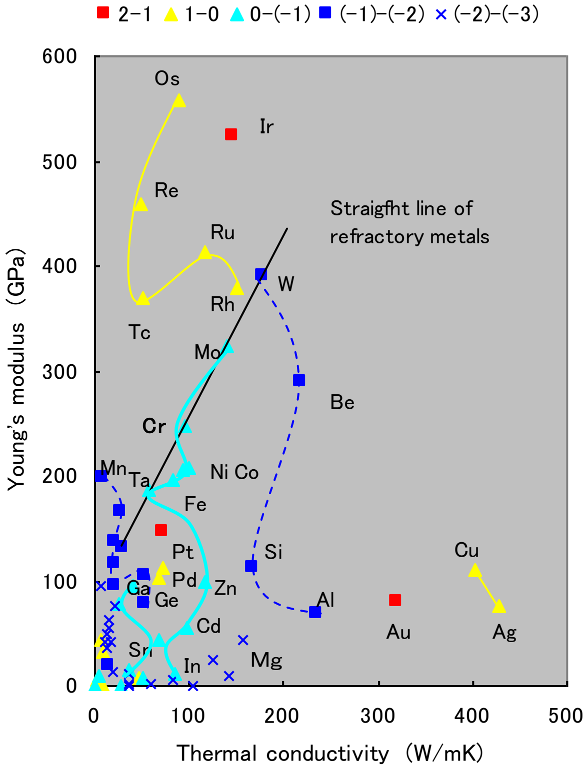

Figure 2: Electrode potential of elements on the TC-YM diagram

B. Electronegativity

The electronegativity shows how easily the electrons are attracted to the atoms in the chemical compounds [10, 11].

The values of the electyronegativity of elements are plotted on the TC-YM diagram and shown in Figure 3.

The general trend which was observed in electrode potential is obscure. The range of the elements with medium electrode potentials is expanded.

Only the elements of larger Young's moduli show large electronegativities. In contrast to the electrode potential, only Au shows a large electronegativity in the high thermal conductivity range. The elements Pt, Pd, and Ge show large electronegativities also in this case. Other elements show medium or small electronegativities.

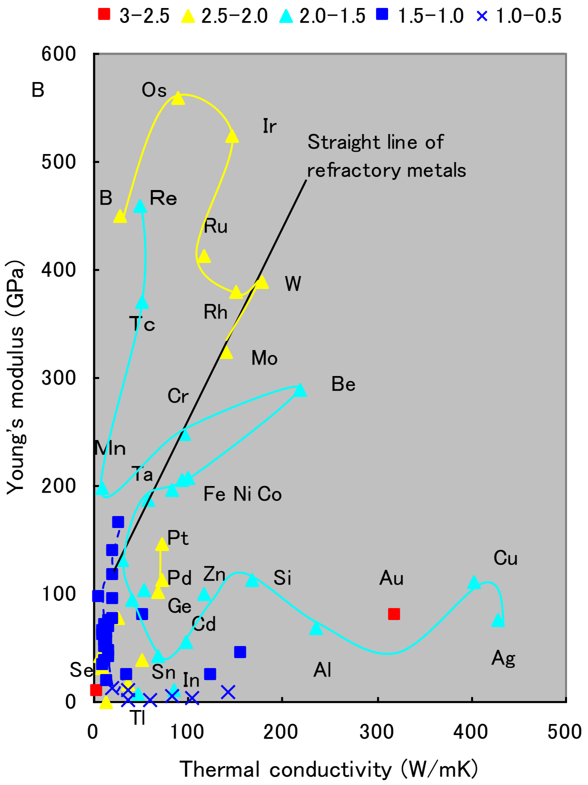

Figure 3: Electronegativities of elements on the TC-YM diagram

C. Ionization energy

The ionization energy means the energy which is needed when an electron is removed from an atom in the gaseous condition.

Figure 4 shows the distribution of ionization energies of elements on the TC-YM diagram. The figures in the legend show the range of ionization energy in units of eV.

The distribution of the ionization energy differs very much from both the electrode potential and electronegativity.

The elements of the highest Young's moduli Ir, Os, and B show large ionization energy. But the most remarkable thing is that many elements surrounding Zn show large ionization energy. This is different from the cases of both the electrode potential and electronegativity.

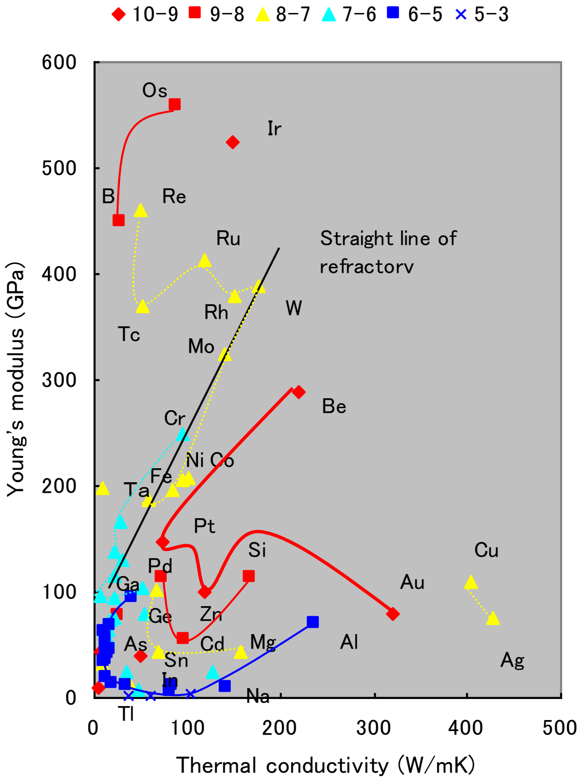

Figure 4: Ionization energy of elements on the TC-YM diagram

D. Electron affinity

The electron affinity means the energy which is needed when an electron is added to an atom in the gaseous condition.

Figure 5 shows the distribution of the electron affinities of elements on the TC-YM diagram. The pattern is basically identical to that of the electrode potential.

The elements of the largest Young's moduli Os, Ir, Ru, and Rh show large electron affinities. The elements around Au also show large electron affinities. Moreover, the elements around Pt also show large electron affinities. The other elements elsewhere show small electron affinities. The most remarkable thing is that the hcp-structured elements Mg, Cd, Zn, and Be show negative electron affinities, forming a deep valley. The elements Mg, Cd, Zn, and Be are the elements which showed the largest ionization energies in Figure 3.

The elements Ir, Au, and Pt show the poles clearly in the electron affinity, identically in the electrode potential, electronegativity, and ionization potential. Therefore, only the elements Mg, Cd, Zn, and Be show the anomaly.

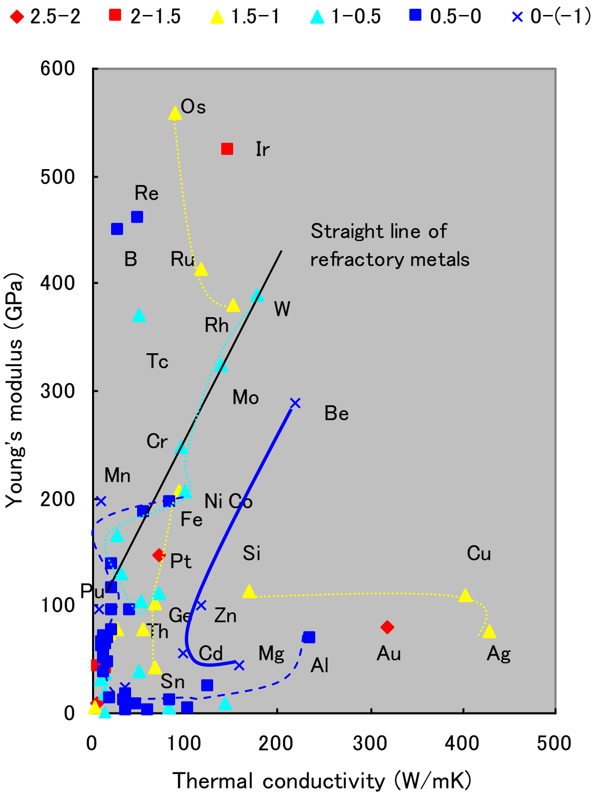

Figure 4: Electron affinity of elements on the TC-YM diagram

III. DISCUSSION

A. Correlation with the periodic table

The electron charge-discharge characteristics have been discussed by means of the periodicity of the elements. Figure 5 shows the electrode potentials of elements on the periodic table. With increasing group number, the electrode potential increases. It drops at the elements of group 12 and 13, Zn, Ga, Cd, and In, abruptly. But in Figure 2, Zn, Ga, Cd, and In are included smoothly in the elements of medium electrode potentials.

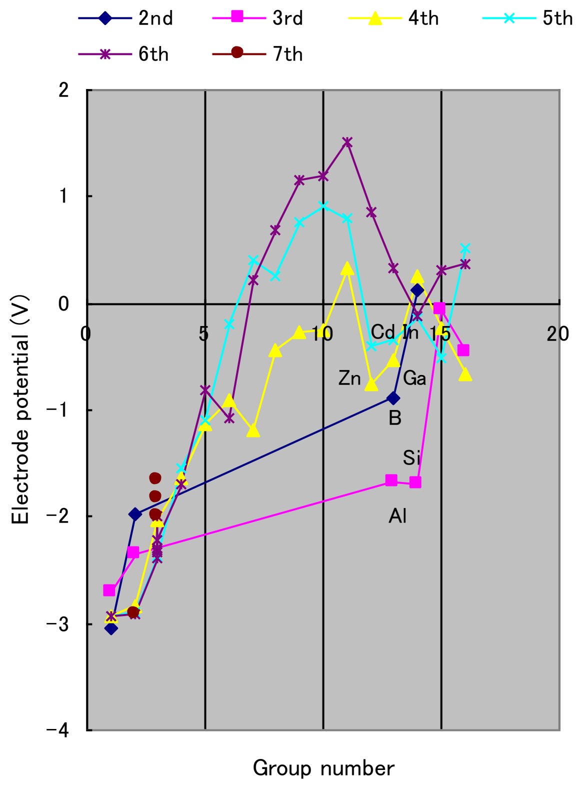

Figure 6: Electrode potentials of elements on the periodic table

Figure 7 shows the electonegativities of elements on the periodic table. With increasing group number, the electronegativity increases. This has been referred to very frequently in books [12,13]. But it is a very rough story. Practically, the electronegativity varies in the complicate way with group number, as shown in Figure 7. It drops at the elements of group 7, Mn, Tc, and Re, and at the elements of group 12 and 13, Zn, Cd, Al, Ga, and In. It is difficult to extract some tendency from these facts. In contrast, these elements are included smoothly in the vast range of the medium electronegativity on the TC-YM diagram in Figure 3.

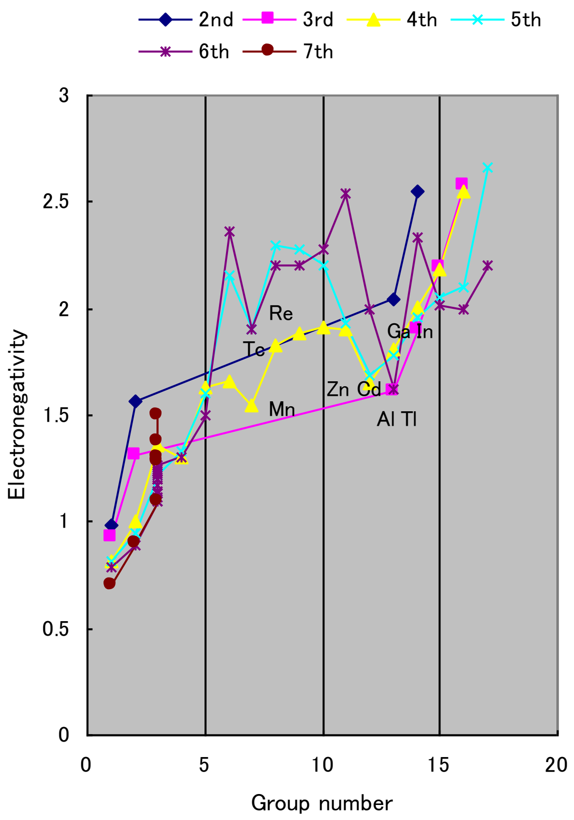

Figure 7: Electronegativvities of elements on the periodic table

Figure 8 shows the ionization energies of elements on the periodic table. With increasing group number, the ionization energy of elements increases. It rises abruptly at Hg, Zn, and Cd, and next drops rapidly at Al, Ga, Tl, and In. It is difficult to explain the rapid change at group 12 and 13. But, in Figure 4, Zn connects to Au, Pt, and Be smoothly, and Cd connects to Si and Pd smoothly, respectively. It is difficult to imagine from the periodic table that Zn is located near Au, Pt, and Be, and Cd is near Si and Pd. This ia the great advantage of the TC-YM diagram.

In contrast, Al, which shows small ionization energy, connects to Na, In, Tl, and Ga smoothly on the TC-YM diagram. It is understandable that Al shows the similar and low ionization energy to Ga, Tl, and In. It can be said that the TC-YM diagram is effective for the explanation of the relationships between the elements.

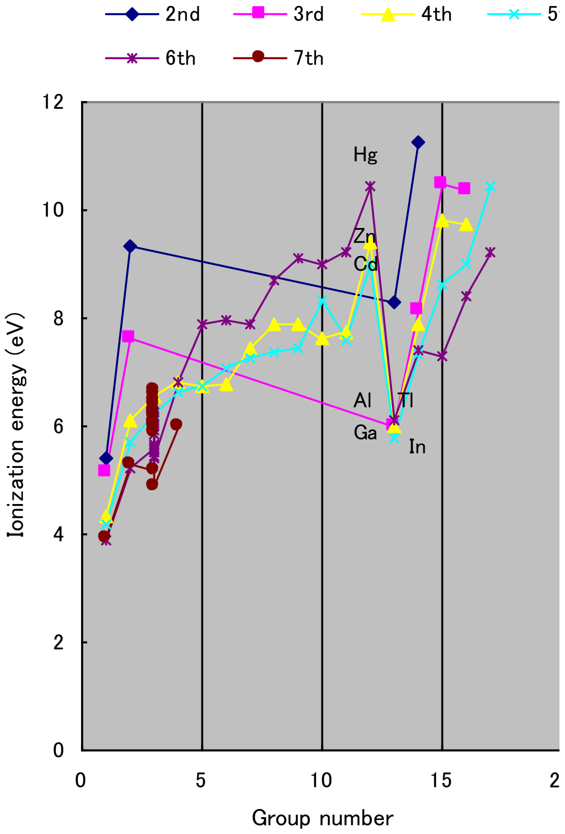

Figure 8: Ionization energies on the periodic tables

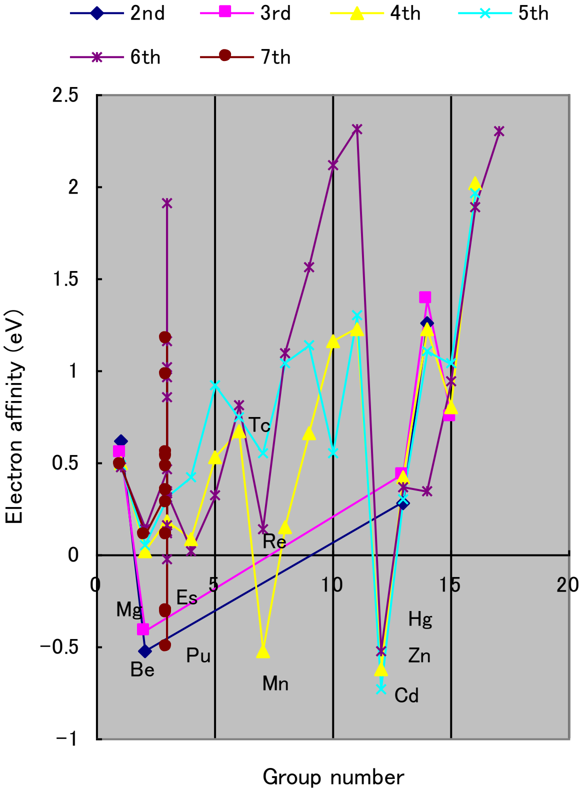

Figure 9: Electron affinities of elements on the periodic table

Figure 9 shows the electron affinities of elements on the periodic table. With increasing group number, the electron affinity of elements increases. But fluctuation is very large, and it is impossible to find out any tendency. But as shown in Figure 5, on the TC-YM diagram, a clean tendency can be recognized.

B. Correlation with the atomic radius

The outer shell electrons are attracted by the protons in the nucleus. Therefore, with decreasing atomic diameter, the electron-discharge characteristics such as electronegativity and ionization energy increase [13-14]. Figure 10 shows the distribution of atomic radii of elements on the TC-YM diagram. The figures in the legend show the range of atomic radius in units of 10^{-10}m. The ionization energy shown in Figure 4 shows the similar pattern to Figure 10.

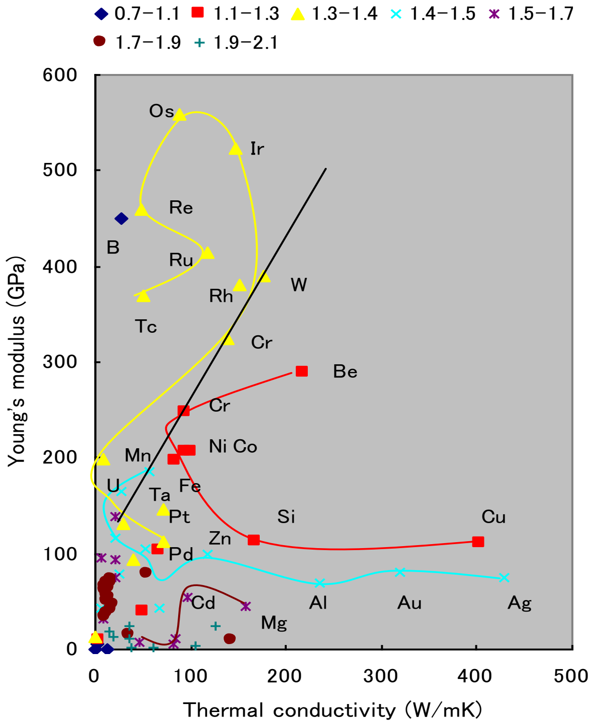

Figure 10: Distribution of atomic radii of elements on the TC-YM diagram

Figure 11 shows the relationship between the electrode potential and the atomic radius of elements. Only a slight tendency is recognized.

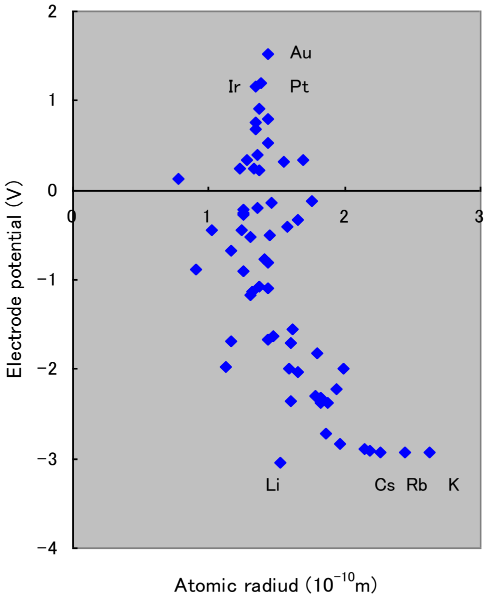

Figure 11: Relationship between the electrode potentials and atomic radius of elements

Figure 12 shows the relationship between the electronegativity and the atomic radius of elements. The situation is very similar to the electrode potential. Only a vague tendency is recognized. This is the Darken-Gurry plot for the explanation of the solubility of elements in metals [1].

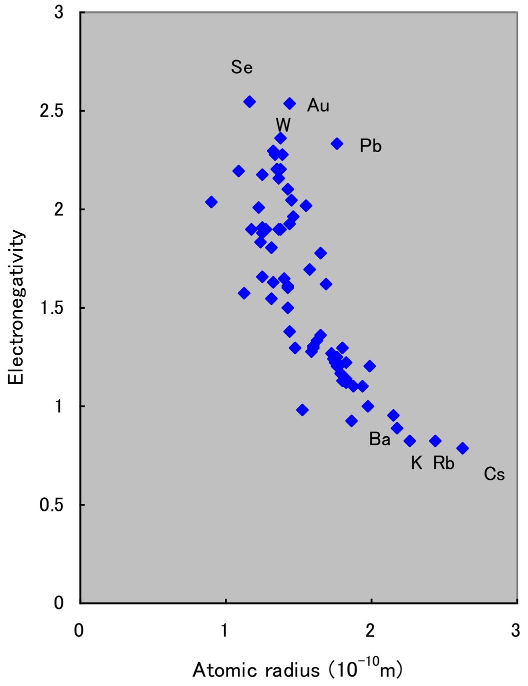

Figure 12: Relationship between the electrode potential and atomic radius of elements

Figure 13 shows the relationship between the ionization energy and the atomic radius of elements. The ionization energy shows the strongest tendency among these characteristics.

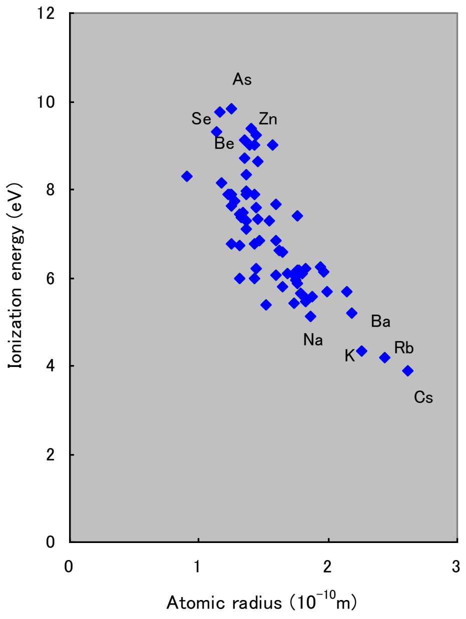

Figure 13: Relationship between the ionization energy and atomic radius of elements

Figure 14 shows the relationship between the electron affinity and the atomic radius of elements. Tendency is not recognized.

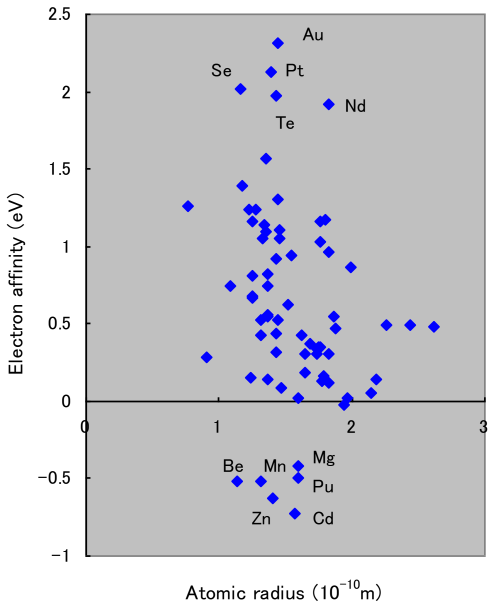

Figure 14: Relationship between the electron affinity and atomic radius of elements

C. *Correlation with the Fermi energy*

From mentioned above, it was found that there are three peaks commonly in the electrode potential, electronegativity, ionization energy, and electron affinity on the TC-YM diagram. They are in the region of largest Young's modulus near Ir, in the region of the largest thermal conductivity near Au, and in the center near Pt, respectively. The elements in those regions show the largest electrode potential, electronegativity, ionization energy, and electron affinity, respectively.

These phenomena may relate to the properties of the electrons on the outer shell of the atom. In general, the Fermi energy expresses the energy of these electrons [15, 16].

The Fermi energy is given in the form of

$$E_F = 0.3646 \times \left(\frac{e/a}{\Omega} \right)^{2/3} \text{ eV}, \qquad (1)$$

where Ω is the volume per atom in units of nm^3 and e/a is the number of the valence electrons per atom [17]. In this way, the Fermi energy is not a base quantity, but a derived quantity. The volume of atom Ω is derived from the crystal structure and lattice constant.

Therefore, the values of the Fermi energy of elements do not show a simple pattern on the TC-YM diagram like the base quantities. Figure 15 shows the distribution of the Fermi energy of elements on the TC-YM diagram. The values of the Fermi energy of elements were adopted from the literature [17]. There can be seen an obscure trend. For the elements of low Young's modulus, with increasing thermal conductivity, the Fermi energy gradually increases, consequently, Cu at the right-most end shows a medium Fermi energy. For the elements of high Young's modulus, with increasing Young's modulus and thermal conductivity, the Fermi energy increases. Be in the high conductivity and high modulus region shows the largest Fermi energy.

Comparing Figure 15 with Figure 2, 3, 4 and 5, it is difficult to speculate correlations between them. Nevertheless, the correlations between them were examined here.

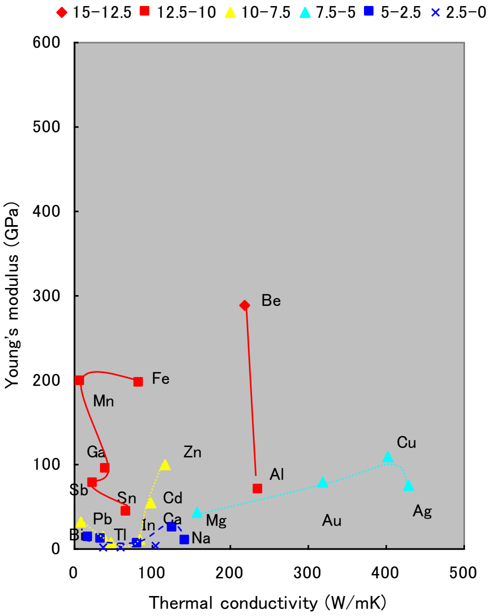

Figure 15: Fermi energies of elements on the TC-YM diagram

Figure 16 shows the relationship between Fermi energy and electrode potential at the elements in which the values of the Fermi energy are available. Surprisingly, the correlation was recognized. But it doesn't have a simple linearity. The electrode potential increases from the smallest Fermi energy and the lowest electrode potential at Cs, Rb, and K up to the elements Al and Be, with increasing Fermi energy, and bends at Al and Be. After that, the electrode potential increases up to Ag, Au and Cu with decreasing Fermi energy. The element groups (Cs, Rb, K), (Al, Be), and (Au, Ag, C) will be used as the landmarks for other figures below.

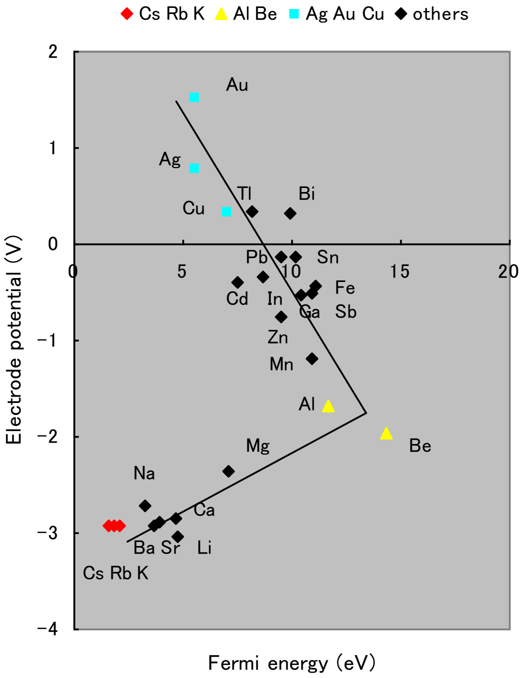

Figure 16: Relationship between the Fermi energy and electrode potential for the selected elements

Figure 17 shows the relationship between Fermi energy and electronegativity at the same elements in Figure 16. Though the basic pattern with the fold is essentially identical to the electrode potential, the scatter is rather large.

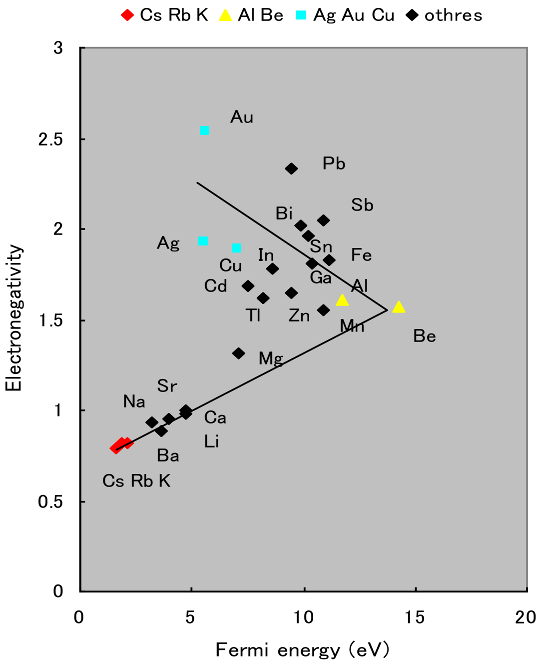

Figure 17: Relationship between the Fermi energy and electronegativity for the selected elements

Figure 18 shows the relationship between Fermi energy and ionization energy at the same elements in Figure 16. The pattern is deformed, and the scatter is large.

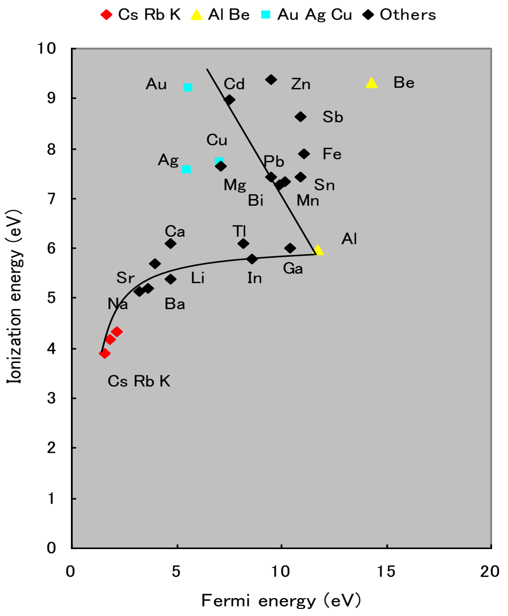

Figure 18: Relationship between the Fermi energy and ionization energyfor the selected elements

Figure 19 shows the relationship between Fermi energy and electron affinity at the same elements in Figure 16. The trends are divided into three ranks. The elements Cd, Zn, Be, and Mg form the lowest rank. The elements Ca, Tl, In, Pb, Ga, Fe, and Al form the second rank. The rest elements form the pattern like other quantities. In this case, the elements Cs, Rb, and K show large values, in contrast to the cases of Figure 16, 17, and 18.

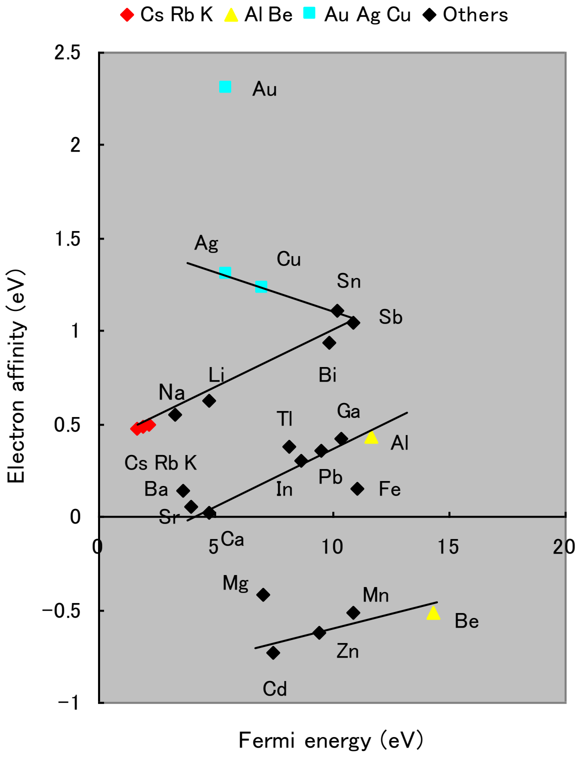

Figure 19: Relationship Between the Fermi Energy and Electron Affinity for the Selected Elements

IV. CONCLUSIONS

The electron charge-discharge characteristics of elements, including electrode potential, electro negativity, ionization energy, and electron affinity, show three peaks on the TC-YM diagram. The first is the region of the highest Young's modulus near Ir. The second is the region of the highest thermal conductivity near Au. The third is the region around Pt near the center of the diagram. The elements Ir, Au, and Pt behave as the poles of these characteristics on the TC-YM diagram.

The electrode potential, electronegativity, ionization energy, and electron affinity show clear patterns on the TC-YM diagram, respectively.

The correlation of these quantities to the periodic table shows no systematic tendencies.

The correlation of these quantities to the atomic radius show very vague tendencies.

The Fermi energy shows the largest values at Be and Ni, which are located in the medium thermal conductivity region on the TC-YM diagram.

Some correlations of the Fermi energy to these quantities were recognized. In the smaller range of the quantities, with increasing Fermi energy, the quantity increases. In contrast, in the larger range of the quantities, with decreasing Fermi energy, the quantity increases. This tendency is the clearest in the electrode potential, and becomes obscurer in the order of electronegativity, ionization energy, and electron affinity.

As a conclusion, the best method to represent the electron charge-discharge characteristics of elements is the expression on the TC-YM diagram. The characteristics of each element connect to each other smoothly on the TC-YM diagram. The elucidation of the mechanism in these quantities is expected.

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