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Materials to Save Humankind and Dreams in my Research

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The basic concept of materials to save mankind sometimes faces to discrepancy with art and politics. "Mottainai" is important. Dreams on the research in computer simulation (molecular dynamics), positron annihilation, high temperature field ion microscopy and transmission positron microscopy are mentioned.

Key words: Materials to save mankind, dreams in research, molecular dynamics, positron annihilation, high temperature field ion microscopy, transmission positron microscopy

1. MATERIALS TO SAVE HUMANKIND

Ages are named by the materials which are widely used by humankind, the Stone age, the Bronze Age, and the Iron Age. In the twentieth century, science and technology have been rapidly developed, compared with preceding centuries. In the twentieth century, metallic materials, ceramic materials, semiconductor materials, organic materials, or composite materials, advanced materials fitting the right materials in the right purpose have been developed. One kind material did not dominate over other materials. In 1950's a field of materials science has been started. Professor Frederick Seitz had the original idea of materials science even during the World War II.

Materials have been developed only to satisfy their purposes. At present, however, due to a rapid increase of the world population (150 persons increase per second [1]), plutocracy, mass production, mass waste, low and natural waste, and enlargement between the rich and the poor people, the concepts of research and development have been greatly changed. The limitation of natural resources and the earth has to be considered. Global warming is one of the most important problems in the present world. The most important point is due to the emission of carbon dioxide to atmosphere from many sources. Energy waste, pollution exhaust fumes, exhaustion natural resources and energy are becoming very serious problems.

Developing materials having good physical and chemical properties is not the final object. This has been clearly shown with the development and accidents of PCB (Polychlorinated biphenyl).

Economy in the twenty first century has to consider limited natural resources and global environment. Materials which minimize natural resources, energy and environmental pollution should be widely propagated. Green products and natural resources are the center of attention. With these properties, high productivity, high recycle performance, minimum burden are demanded. The life cycle assessment (LCA) covers from mining, extraction, row materials, processing, use, to waste including energy consumption and recycles. The concept has been changed in forty years, from diversification to unification in materials. The present author proposes a model of double helices as shown in Fig. 1. Process, structure, properties, performance and functions are on one helix, and life cycle assessment, safety, environment, product responsibility are on the other helix. Evaluations are connected these two helices. Population increase, waste of natural resources and waste of energy pull down the whole system, on the other hand, researches beneficial to mankind pulling up the whole system. We hope the helices go up and up.

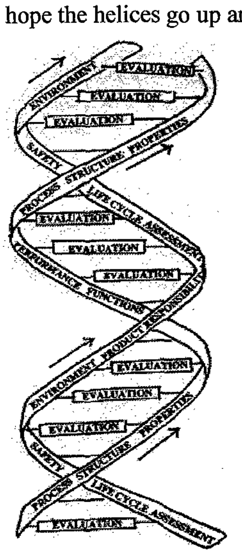

Fig. 1. Double helices of materials science.

We should spread "MOTTAINAI" (save, opposite of wasteful) spirit. Do not waste. "Stint ourselves in everything" should be considered as a virtue. "Increase GDP!" or "Increase individual consumptions!" is inconsistent with "Saving from human crises". Japanese government encourages for people to increase consumptions to keep good economy situation. The government is encouraging to buy things not really needed, then the government says, "business will be brisk". This is against saving mankind. Creation of world new economy system is necessary. How can we eliminate discrepancy? Spendthrift habit should be purged. "MOTTAINAI" Niggardliness is not only for saving money but also saving humankind.

1.1 Discrepancy with art and politics

How efficiency comes in the field of arts? We have to devote much time to do something better. Evaluation of art is the evaluation of product, not the process or efficiency which is important factor in engineering. These concepts sometimes have discrepancies with human civilization and cultures. For example, to make good Japanese Sake, sixty per cent of rice is polished off, otherwise good sake cannot be produced. On the other hand, there are many children who are dying by hunger every day in the world. Should we satisfy poor sake made from whole grains of rice? Which is eco-materials? Which is art?

Cabbages are produced too much in certain years in Japan, farmers destroy cabbages by tractors. Then the Japanese government gives subsidies to the farmers. Is this right? Something wrong! In Japan, if farmers do not grow rice in their rice field, they get subsidies from the government. Bent cucumbers are unable to sell and are thrown away. Japan only produces 40 per cent of the food needs, the rest is imported. I hear French government subsidies wine glowers if they through away wine. Such policies are the ruin of humankind. Don't you think something wrong?

When I have been to the U. S. A. first in 1954, I was astonished to find an advertisement saying "The more you use papers, the more you support paper industry". I was surprised to find a sugar pot was on a table in restaurants. Sugar was rationed in Japan at that time. I could not imagine we can use sugar as much as we wanted.

It is cheaper to buy a new appliance instead of repairing it now. Broken electric appliances are not repaired, because repairing is more expensive than buying new ones. We can save money but we waste resources, waste effort to make. People only care saving money. Mass production reduces the production cost but during the development, much effort and materials and energies were used. The present flow follows mass production.

Now setting the exhaustion quota of CO_2 is difficult. Many crises can be solved if the human population does not increase in the world. Can we set population quota? This is much more difficult problem. Population control, however, solve all the present problems.

Fossil fuels should be used for more useful purpose such as making chemical materials other than fuels. Atomic energy is dangerous, but probably energies will be supplied by atomic energy even though it has danger. This is contradictory to the traditional economy. We have to do something before too late to save humankind. Any kind of species die out. No exceptions. It may be too late?

2. DREAMS IN MY RESEARCH

When I was enrolled in the graduate school of the University of Tokyo, Professor Sanichiro Mizushima sent a letter to the Head of the Department, if he could recommend someone to study under Professor Kuzynski at the University of Notre Dame. I was selected for this opportunity. This was the largest turning point in my life.

2.1. University of Illinois

After I received Master of Science in Metallurgy from Professor Kuczynski, I transferred to the University of Illinois at Urbana-Champaign by Professor Seitz's kind invitation. Quenching of pure silver to measure the formation energy of a vacancy in silver was my Ph. D. thesis theme [2,3]. At that time, atomic reactor was not allowed to build in Japan and Japan was a poor country, no use to study radiation effects. I worked under Professors Seitz and Koehler, a Mecca for the study of crystalline defects. We have shown that Stage III recovery of aluminum after low temperature electron irradiation was due to the recovery of vacancies [4,5]. I was the first one to move into the Loomis Laboratory (New Physics Building) at the University of Illinois during construction and we were the first one to use Van De Graaf newly introduced to the basement of Frederick Seitz Laboratory at U. of I. The electricity was accidentally cut off from time to time, and the diffusion pump oil had to be changed during construction of Loomis Laboratory. After received Ph. D., I quenched aluminum dilute alloys to study the recovery.

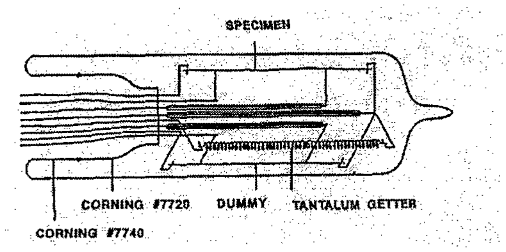

Fig. 2. Glass tube for quenching pure silver.

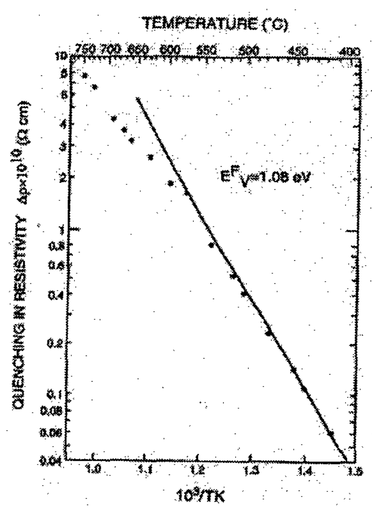

Fig. 3. Quenched in electrical resistivity vs. quenching temperature.

2.2 Argonne National Laboratory

I moved to Argonne National Laboratory to receive my immigrant visa. While I was waiting experimental apparatus to come, I started to study crystalline defects using computers with Rod Cotterill. The time we started the work, the newest computer was still primitive. Meanwhile a CDC3600 computer was delivered to Argonne. We were the first one to simulate dislocations in the three dimensions in the world (Fig. 4) [6]. We have shown that complete dislocations need no activation energies to split and connected with a stacking fault. This had been a puzzle since my graduation thesis at the University of Tokyo. Figure 5 is the core energy within a radius r from the center of an edge dislocation vs. r. Core energy of dissociated dislocation is the least in elasto-atomic, complete and dissociate dislocation follows. At that time it was said that atoms in a core of dislocation are melted or hollow.

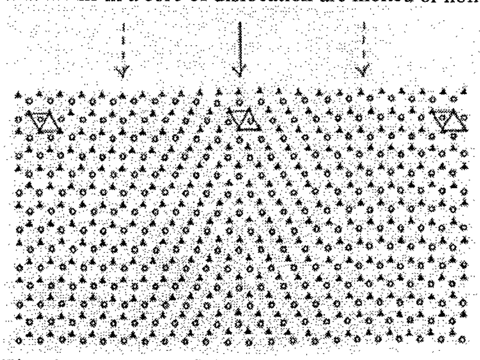

Fig. 4. Projection of three layers atoms on (111) of a dissociated edge dislocation in copper.

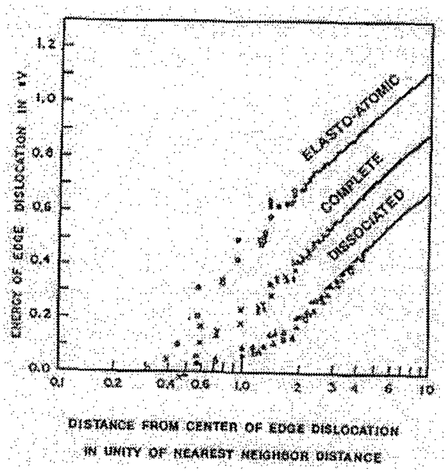

Fig. 5. Energies of an edge dislocation (elasto-atomic, complete and dissociated dislocation) within radius r vs. distance r from the center.

Professor R. R. Hasiguti, my adviser at the U. of Tokyo, asked me if I was interested in joining the University of Tokyo as an associate professor under him when I saw him at the International Conference on the Study of Lattice Defects and Diffraction held in Melbourne, Australia in 1965. I accepted his offer. I told Dr. O. C. Simpson, the Director of the Solid State Science Division, Argonne National Laboratory that I wanted go back to the University of Tokyo. He offered me the same salary I would get in Japan. I told him that my salary would be one tenth of the salary I was getting at Argonne. Then he asked me if I would be the Director of the Faculty of Engineering. I answered him that I would be an associate professor. He said that I was crazy. He gave me "On leave" status. I thank to Dr. Simpson.

2.3 Positron Annihilation

After I came back to Japan, I wanted to start a new experiment. The Fermi surfaces of concentrated alloys were difficult to measure at that time. Positron annihilation technique is one of the most powerful methods. So I had Susumu Nanao (now a professor at the University of Tokyo) visit Professor Kunio Fujiwara. Fortunately INCRA (International Copper Research Association) gave me US$3,000 a year for three years. This was the start of our experiments with devoted associates and students including Shoichiro Tanigawa. Nanao told me that the angular correlation curves of annihilated gamma rays were different after successive neutron irradiations [7]. We could not make new single crystals of Cu-Ni alloys, we had to send the same specimen back for neutron irradiation to form ^{64}Cu in the specimen itself. I felt a cold chill passed through me when I heard Nanao's word. I thought this was due to the vacancy clusters made by neutron irradiation to form ^{64}Cu in the specimen itself. Since this one word, we have concentrated studying crystalline defects and phase transitions by positrons [8]. Positrons are trapped by vacancies. Neutron irradiation accumulated more vacancy type defects. One of the best measurements is shown in Fig. 6 [9]. The positron lifetime extended in Stage III in copper after low temperature irradiation. This clearly shows that vacancies move in Stage III forming larger vacancy type defects, not interstitials are moving.

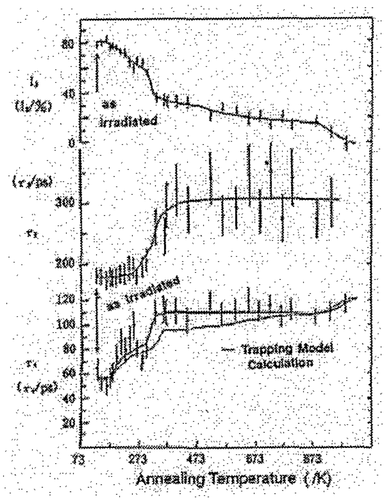

Fig. 6. Positron lifetime in copper during iso-chronal annealing after electron irradiation at liquid nitrogen temperature.

Tanigawa et al irradiated pure iron at liquid nitrogen temperature by neutrons and measured positron lifetime during iso-chronal annealing. The lifetime was extended near 180K and concluded vacancies in pure iron move near 180K. At that time people believed that vacancies in iron move at 200°C. We were claimed our talk at the Physical Society of Japan Meeting, the publication was delayed [10]. Fukushima and Doyama have found that the formation energies of a vacancy in copper alloys are linear with the electron to atom ratio (Fig. 8) [11,12]. Figure 9 shows that the apparent formation energies of a vacancy in copper alloys are linear with the Fermi energy and are also linear with atomic concentration of alloying element/solubility limit [12].

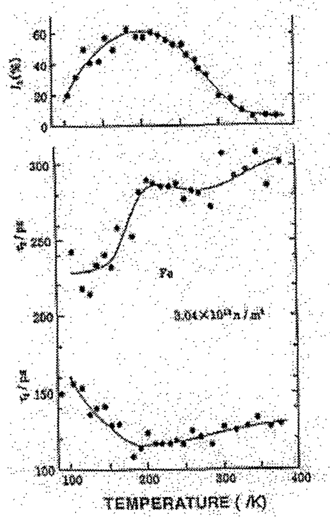

Fig. 7. Positron lifetime in iron during iso-chronal annealing after neutron irradiation at liquid nitrogen temperature.

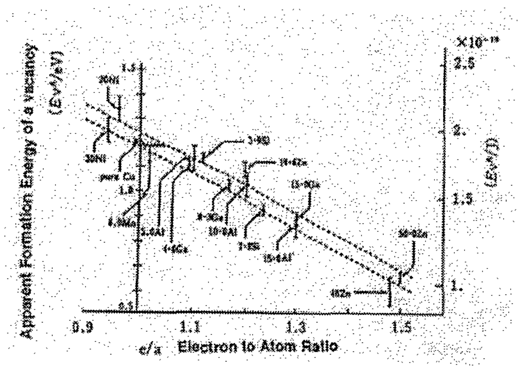

Fig. 8. Formation energies of a vacancy in copper alloys are linear with the electron to atom ratio [11].

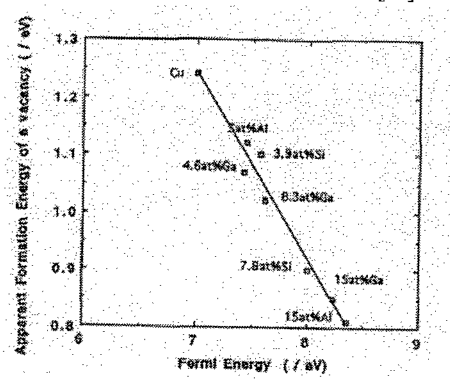

Fig. 9. Formation energies of a vacancy in copper alloys are linear with the Fermi energy. [12].

2.4. High Temperature Field Ion Microscopy

Ishimoto accidentally observed images of atoms of a specimen in a field ion microscope while the specimen was heated. He saw atom images even at red hot temperatures through a channel plate [13]. As everyone knows the atom images can be only observed at the temperature of a specimen lower than liquid nitrogen temperature with imaging gas. Latter we saw atoms running on a specimen surface at red hot temperatures without imaging gas (Fig. 11) [14]. This was also unexpected.

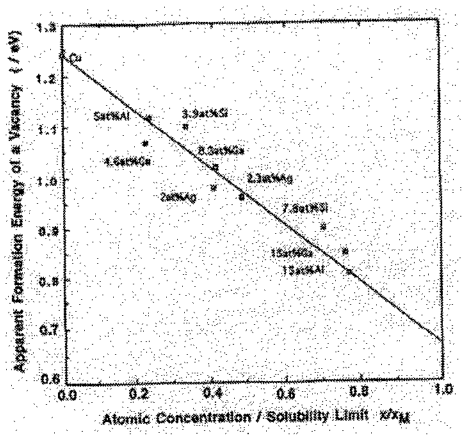

Fig. 10. Formation energies of a vacancy in copper are linear with atomic concentration / solubility limit [12].
2.4 High Temperature Field Ion Microscopy

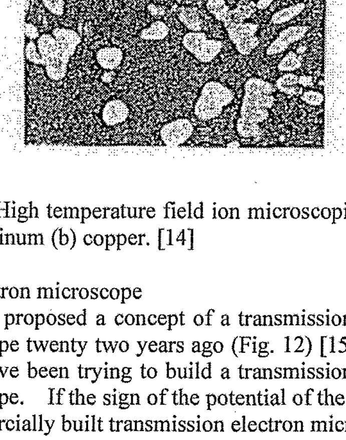

Fig. 11. High temperature field ion microscopic images. (a) Aluminum (b) copper. [14]

2. 5 Positron microscope

I have proposed a concept of a transmission positron microscope twenty two years ago (Fig. 12) [15]. Since then I have been trying to build a transmission positron microscope. If the sign of the potential of the source of a commercially built transmission electron microscope is

reversed and a positron beam is supplied, positron images can be obtained. The intensity of a positron beam is the key to solve this problem. The high intensity positron beam can be obtained by an accelerator or an atomic reactor. The most essential point is to obtain a research fund.
More than twenty years ago, the research aid situation was not good in Japan, and on the first page of application form we have to write the age of the applicant in Japan even now. I have received continued

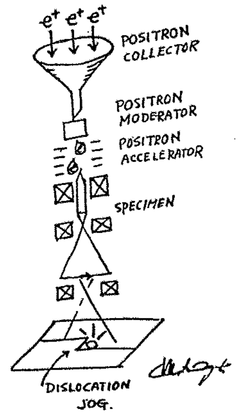

Fig. 12. A concept of a transmission positron microscope [15].

research aids, not much but continuous from Ministry of Education, I thank to MEXT and referees for their warm support. Positron beam was also not ready at KEK. In 2005, Professor Fujinami granted a large fund sponsored by the Japan Science and Technology Agency (JST) and the project is going now. I am also a member of the project. We hope to obtain positron images soon.

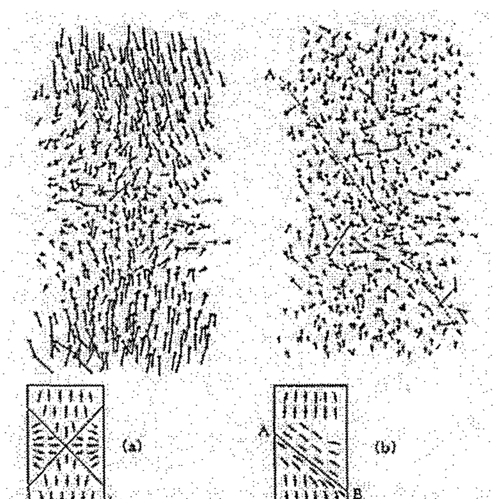

Fig. 13. Plastic deformation of amorphous iron. (a) Elastic region, (b) plastic region, atoms above and below Plane AB, move opposite direction, a dislocation like can be observed [16].

2.6 Computer simulation
Another project I have been involved is molecular dynamic using computers. When I came back from the U. S. A. Hitachi made a high speed computer HITAC but took us a few days to debug, compared with less than 10 minutes at Argonne National Laboratory. I did not work molecular dynamics at the University of Tokyo at that time. Meanwhile a fifteen year old FACOM in the Faculty of Engineering was given away. I got it free of charge, but I found that the maintenance fee was six million Japanese yens a year, even only the essential parts were operating. Professor Moto-oka, a professor in Department of Electrical Engineering introduced me to Mr. Takuma Yamamoto in Fujitsu. I negotiated to pay two million Yens a year and I was happy. He became the President of Fujitsu latter and he made a successful bid for the Complete Computer System of Hiroshima for 1 yen, I should have asked also 1 yen to Mr. Yamamoto. So Ryoichi Yamamoto can use the computer for 24 hours a day. We could calculate the atomic position of amorphous iron and even the plastic deformation of amorphous iron which could not performed without the FACOM [16]. I nicknamed the old FACOM "Old Jacqeline (Kennedy Onassis)", which means it costs a lot only keeping her.

The interaction potential has been changed from pair potential [16] to many body potential [17] . We have been using embedded atom potentials. We have shown that dislocations are created near the tip of a notch in tensile test. We have shown the projection of atomic positions (upper figures) and simulated images of Lang method (lower figures)[18] during plastic deformation of copper single crystals. A rectangular parallelepiped copper single crystal specimen, surrounded by (00-1), (001), (0-11), (01-1), (011), with a notch on (001) was prepared. The crystal was pulled in [011] direction. During tension, positions of atoms near the center plane are plotted on (0-11) upper plots of Fig. 14.

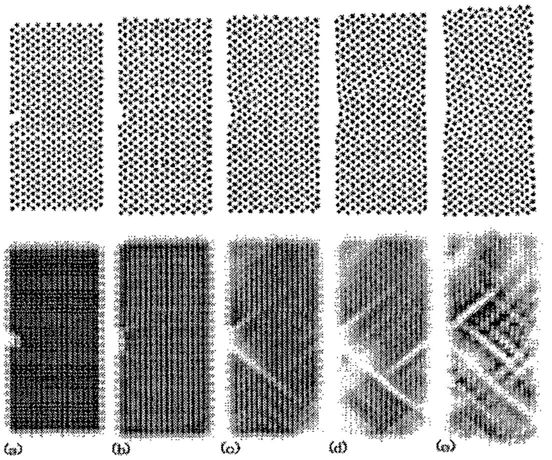

Fig. 14. A copper single crystal was pulled in [011] direction. (a) positions of three atomic layers near the center were projected on (001), (b) corresponding simulations of Lang photographs are plotted.

Lower plots are Lang photograph simulation corresponding to the upper states. In lower plots, it is clearly seen dislocations were created near the tip of the notch. Figure 15 corresponds to Fig. 14 (c). Upper half figures are before deformed, and lower half figures are the state of Fig. 14 (c). The crystal is rotated until (111) plane becomes vertical. Three atomic layers near a slip plane was plotted lower right. A pair of partial dislocations connected with a stacking fault can be seen in the lower right figure.

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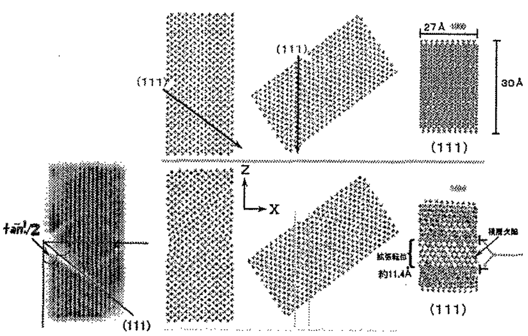

Fig. 15. Upper half is the projection of atomic positions on (001) before pulling (left figure). The crystal was turned so that the slip plane (111) becomes perpendicular (middle). Three atomic layers are plotted in the right figure. Lower half is corresponding Fig. 14 (c). In the figures of lower half are corresponding to upper half. Low right figure, partial dislocations can be seen.

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