Proceedings of the 12th International Conference on
Aluminium Alloys, September 5-9, 2010, Yokohama, Japan

pp. 1397-1404

Towards Innovation in Materials Design for Aluminum Alloys with First Principle Calculations

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Understanding on the mechanisms of strengthening and fracture, is one of the most important topics in the research field for metallic materials science, has been carried out by phenomenological approach with particular emphasis on mathematical formulation and practical investigations. Now the topics should be rather physically motivated as to deal with the physical background of the materials subject to deformation concerning to strengthening and fracture. The topics especially devoted to the actual deformation mechanisms and their interrelationship with not only the materials design but also the materials processing with the microstructure controlling. The essential knowledge in nano-scale, including an atomistic mechanism of strengthening and fracture, is in great demand not only from scientists but also from engineers. Therefore the mechanisms of strengthening and fracture have been reexamined by the knowledge and understanding from the results by the first principle calculations. As examples the misfit strain of the solute atoms in aluminum is calculated in order to identify the elements to make the strength of the binary aluminum alloys much more higher. Furthermore, the grain boundary segregation energies of the solute atoms in aluminum are calculated in order to investigate a tendency of the segregation of the solute atoms around grain boundary, which might affect the critical strength of the intergranular fracture for the aluminum based alloys. Finally, author will try to describe the personal view and opinion on future directions in materials science research by summarizing the outline of the results in the recent works by the first principle calculations on the atomistic scaled strengthening and fracture mechanisms.

Keywords: *Misfit strain, Grain boundary segregation energy, Surface segregation energy, Strengthening mechanisms, Fracture.*

1. Introduction

From the recent opinion on the trends and limitation of the research in structural materials, which has been reported in a literature [1], the studies can be divided into two categories, one is the basic and scientific studies on materials design and the other the application of the materials processing to commercial forming or its related processes. It has been often pointed out that an advancement of the commercial applications is crucial for future activities in research field to structural materials. By taking into account the past advancement on the researches of the structural materials, the following research topics might have been considered to be important, or were settled at the onset of the desired future researches.

1. Discovery of the new structural materials (nano-scaled structural materials, non-equilibrium materials, bulk metallic glasses, room-temperature high-strain-rate superplastic materials, ultra light materials etc.)
2. Grain boundary plasticity (fracture, grain boundary segregation, grain boundary sliding, grain boundary structure, grain boundary chemistry etc.)

3. Basic engineering applications (micromechanics, highly straining materials processes, new specific forming and joining processes etc.)

In the first topic it is believed that the future development in the structural materials research field depends on whether new performance or phenomena in materials or an attractive topic including engineering application can be discovered steadily. This was the common target for all the researchers in materials science. Second, it has been accepted at time that as the recent materials have been a finer structure, grain boundary plasticity has become a new concept of the reliability against fracture and a fundamental process for materials flow during deformation in fine-grained materials exhibiting very high strength or superplasticity. Now the investigation on grain boundary plasticity from atomistic level has been likely to be an effective way to break through the limitations of the macroscopic analysis based on the co-relationship among stress, strain and strain rate. It is very important to note that the atomistic mechanism of not only crystalline plasticity but also grain boundary plasticity is understood differently from a scientist to another. Analysis of grain boundary and its related phenomena from an atomistic level may be effective to form a common view on grain boundary plasticity, and to clarify its atomistic mechanism. Last, engineering application must be very important for future advancement in the field of the structural materials as has often been pointed out so many times in a series of the meetings in Japan.

Mechanisms of the deformation concerning to strengthening and fracture can be studied from different viewpoints, which may be divided into two general categories emerging from the vast content of crystalline plasticity and/or grain boundary plasticity. One is the phenomenological approach with particular emphasis on the mathematical formulation and practical applications. The other is rather physically motivated as to deal with the physical background of materials subject to crystalline plasticity and/or grain boundary plasticity, especially devoted to the actual deformation mechanisms and their interrelationship with evolution of the structure during plastic flow of the materials. Now and also in the near future the essential knowledge of micro/nano-mechanics, including an atomistic mechanism of crystalline plasticity and grain boundary plasticity, is in great demand not only from scientists but also from engineers. As a central link between micro/nano-and macro-scales, however, meso-mechanics aims at introducing the essential micro/nano-mechanics concepts to various intermediate scales where the quantitative theory of the continuum mechanics is still applicable in describing the evolution of the material microstructures during plastic flow. Meso-mechanics represents an important connection between the continuum-based macroscopic-mechanics and the atomistic physical theory of micro/nano-mechanics. The connection here should be in both length scales and the method of investigations.

It is noted that the researches on mechanisms of strengthening and fracture have been advanced in recent ten years by the excellent performance in high resolution ability of analyses by the highly advanced efficient electron microscopes in new materials such as nano-scaled structural materials or non-equilibrium materials, and also by the challenge to timely topics such as the first principles calculations. The discovery of new phenomena and analysis method has been particularly important to keep the activity as high as possible. Author believes that a new area created by meso-mechanics stimulates a close workmanship among metallurgists, mechanists and engineers, and promotes a combined approach of solid mechanics and material science. In this paper, therefore, the outline of the recent results in my laboratory will be summarized from the viewpoints of micro/nano-, meso- and macro-scales on mechanisms of strengthening and fracture. Finally I will try to describe the personal view and opinion on the future directions in researches on mechanics or strength of the metallic structural materials.

2. Calculation Method

The first-principles calculations were performed using the Cambridge Serial Total-Energy Package [2], was an ab initio pseudopotential method code for the solution of the electronic ground state of periodic systems with the wave functions expanded in plane-wave basis using a technique based on

the density functional theory (DFT) [3,4]. The electronic exchange-correlation energy was given by the generalized gradient approximation (GGA) (PW91) of Perdew et al. in the DFT [5]. Troullier-Martins and ultra-soft pseudopotentials were used for aluminum and for other elements, respectively. A Gaussian smearing of 0.1 eV was applied to the occupation numbers. The cut-off energy of 350 eV for plane-wave basis was used. The stable atomic configurations were obtained through relaxation according to the Hellmann-Feynman forces. The lattice constants at zero pressure were optimized using a Broyden-Fletcher-Goldfarb-Shanno (BFGS) minimization algorithm [6].

A supercell containing 125 atoms which was periodic in all three directions was employed for studying the misfit strain in aluminum solid solutions. The supercell contains one substituted solute atom per cell and corresponds to 0.8 at% dilute solid solution. The energy integration over a Brillouin zone was made with k-point grids according to the Monkhorst-Pack [7] sets of 2x2x2 k-points. The misfit strain was derived from a fractional distance between each solute atom and solvent aluminum atom at the first nearest neighbor site.

The formation of grain boundary and surface led to increase lattice strain and supercell volume. Hence, the total energy was minimized with respect to the position of the atoms in the supercells (atomic relaxation) and the lattice constants of the supercells (volume relaxation). The energy integration over a Brillouin zone was made with a k-point grid according to the Monkhorst-Pack set of 4x1x6 k-points together with thermal smearing (k_BT=0.2 eV). The calculated $\Sigma 11(1\bar{1}3)$ [110] (θ =129.52°) tilt grain boundary was constructed using the coincidence site lattice model. This boundary is modeled in the orthorhombic supercell of the bicrystal containing 44 atoms. When $\Sigma 11(1\bar{1}3)$ [110] tilt grain boundary fractures ideally, $(1\bar{1}3)$ free surface is formed as a fracture surface. Calculations procedures in detail as to misfit strain around one substituted solute atom in solid solution and the computational models of a single crystal and a slab containing the two fracture surfaces are described in the previously published literatures [8-11].

3. Micro/Nano (Atomistic) -Scaled Mechanisms

Prediction from the first-principles calculations constructs the physical knowledge to understand the mechanisms of the solid solution strengthening which is one of the important strengthening ways in the non heat-treatable aluminum alloys. Magnesium, zinc, manganese and copper etc. are typical additional elements for the purpose of the solid solution strengthening in commercial aluminum alloys. The effect of the solute atoms on the solid solution strengthening in aluminum alloys has been well investigated by the experimental approaches mainly. Therefore, it is interesting to clarify theoretically an existence of the other elements that are more effective to increase its strength in the solid solute aluminum alloys than the conventional elements used previously in commercial aluminum alloys. The origin of the strengthen mechanisms due to the solid solution is the size mismatch between one solute and the solvent atoms gives a rise to a distortion of the surrounding lattice, is called the misfit strain commonly.

In commercial aluminum alloys, on the other hand, the intergranular fracture due to the grain boundary embrittlement has been discussed from a view of the segregation by alkali metals to grain boundaries, and it was concluded that the trace alkali metal impurities would segregate at grain boundaries and lower the grain boundary cohesion [12,13]. Only a few research has been investigated the grain boundary characteristics and the grain boundary cohesion using the first-principles calculations [15-17], indicating that the ideal tensile strength of the grain boundary is reduced with grain boundary segregations of both Na and Ca [18]. So it is worthy to investigate the energy of the grain boundary segregation of the solute atoms at symmetric tilt $\Sigma 11(1\bar{1}3)[110]$ grain boundary in aluminum alloys from the first-principles calculations. Furthermore, the effect of the grain boundary segregation by the solute atoms on the grain boundary embrittlement in aluminum alloys will be discussed on basis of the model proposed by Rice-Wang [19].

3.1 Misfit Strain

The values of the misfit strain for 55 solute atoms in the aluminum-based binary alloys, as shown in Fig.1, were obtained from the first-principles calculations. The high values more than 6 % in positive are obtained in the elements of Sr, La, Rb, Ba and Cs and a maximum value is about 8 % at an element of Cs, and also the relatively high values about 4 % in misfit strain are achieved in the elements of K, Ca, Y, Tl, Bi, Te, Pb and Po. On the other hand, a maximum value in negative for misfit strain is about 4 % at the element of Fe. Actually it is a common fact for all the elements exhibiting the high values in misfit strain that they are not solute or have quite low solid solubility limit in aluminum (usually less than 0.05 at%, except of Pb at 0.19 at%). Therefore, the non-equilibrium processing such as rapid solidification or vapor quench must be established when the supersaturated solid solution in aluminum could be required by the specific element such as Fe might be much more effective to increase the strength in solid solution.

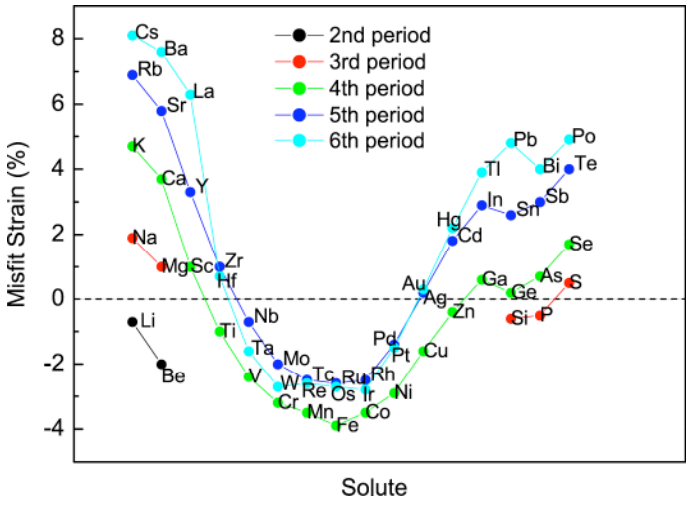

Fig.1 The values of the misfit strain for 55 solute atoms in aluminum-based binary alloys were obtained from the first-principles calculations.

3.2 Fracture Criteria from Grain Boundary Segregation Energy

The effect of the solute atom segregation on the grain boundary cohesion in aluminum was investigated based on the thermodynamics theory after Rice and Wang [19]. The theory suggests that the potency of the solute atom in reducing the Griffith work of a brittle boundary separation is a linear function of the fracture criteria such as $(\Delta E_b - \Delta E_s)$, where ΔE_b is the grain boundary segregation energy of the solute atom, ΔE_s is the surface segregation energy of solute atom respectively. If one solute atom occupies a substitutional position at the grain boundary core, its potency to the embrittlement is then determined by $(\Delta E_b - \Delta E_s)$. If $(\Delta E_b - \Delta E_s) > 0$, the solute atoms would tend to segregate to a free surface rather than a grain boundary, and thus its segregation would make the grain boundary more brittle, then it becomes easy to lead the brittle intergranular fracture. The calculated values of $(\Delta E_b - \Delta E_s)$ are indicated as a function of the element in solid solution in aluminum, shown in Fig. 2. For example, iron might has a high potential to increase the strength in aluminum based materials due to high value in misfit strain, as shown in Fig.1, its value of $(\Delta E_b - \Delta E_s)$ is very close to zero, which clearly indicates that iron atom acts as be almost negligible as an embrittler around the grain boundary. Furthermore, iron showed the positive

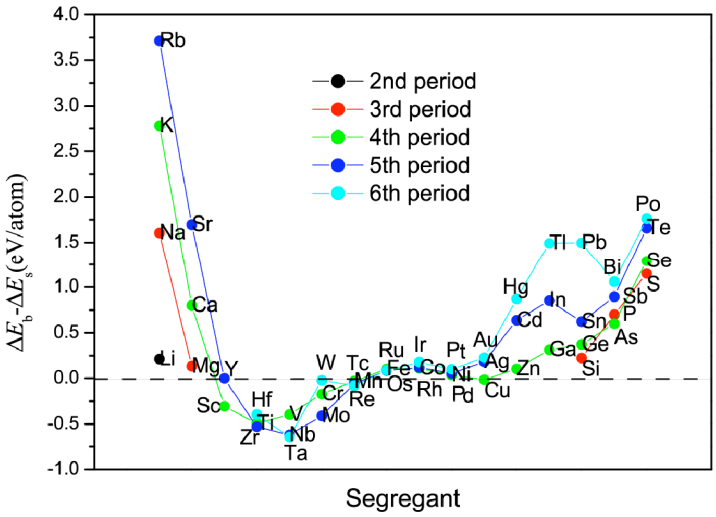

Fig.2 The change of the criteria of grain boundary fracture such as $(\Delta E_b - \Delta E_s)$ against segregants in aluminum-based binary alloys was analyzed from the segregation energies on grain boundary and surface were obtained from the first-principles calculations.

values in grain boundary segregation energy at 0.26 and 0.01 eV/atom in each case of the first or the second nearest neighbor site. That is, most of solute iron atoms would not be segregated on the grain boundary from the result of these positive values in segregation energy, which means that iron atom does not prefer to occupy in the grain boundary in aluminum.

3.3 Element Strategy and Green & Sustainable Metallurgy

Diminishing resources of rare but industrially important elements and the resulting need for a national strategy on rare elements are often discussed. Indeed, metallurgy often relies on rare and precious elements. Avoidance of the rare elements in metallurgy therefore is the way to follow for the sake of national security of Japan. Avoidance of the use of the rare elements, that is, the use of the ubiquitous elements (carbon, iron, aluminum, magnesium, silicon, and calcium), also contributes immensely to conservation of the environment. Iron is obviously more environmentally benign than other elements in aluminum alloys, but replacement of the used other elements by iron needs alchemy by the first-principles calculations. Strategic consideration of the nature of elements, element strategy, must therefore be considered explicitly in research of materials science. How nice it would be if all the structural materials were achieved only with readily available, ubiquitous elements! Element strategy is the common key word for green & sustainable metallurgy. Now it can be concluded that iron is one of the best elements to increase its strength in aluminum without grain boundary embrittlement from prediction by the first-principles calculations.

4. Meso-Scaled Solid Solution Strengthening Mechanisms

The misfit strain of each solute atom in aluminum from the first-principles calculation is summarized in Fig. 1, by which the contribution to yield stress due to the solid solution strengthening can be calculated through the dislocation theory. In Cottrell's procedure with Friedel's theory [20-21] the increment in yield stress due to the solid solution strengthening in a polycrystalline alloy, $\Delta\sigma_s$ is obtained as follows

$$\Delta\sigma_s = M\frac{3^{3/4}}{2}\left(\frac{1+\nu}{1-\nu}\right)^{3/2}\mu|\varepsilon|^{3/2}\sqrt{c} \tag{1}$$

where $\Delta\sigma_s$: the increment in yield stress, μ : the shear modulus, ν : the Poisson's ratio, M : the Taylor factor, ε : the misfit strain, c : the solute concentration.

The yield stress increases as the absolute value of the misfit strain. The calculated values of the increment in yield stress by solid solution strengthening are in good agreements with the reported experimental values in Al-Cu, Al-Mg, Al-Ga and Al-Zn alloys [22], as shown in Table 1. These agreements provide a confidence in the current computational approach. The most effective alloying elements for solid solution strengthening may be expected to be manganese, magnesium, zinc, lithium, and copper in aluminum when the conventional equilibrium processes such as an ingot metallurgical processing could fabricate the aluminum alloys. These elements to be expected by the first-principles calculations are very popular to use commercially in industry scale.

Table 1 Comparison between the calculated values ($\Delta\sigma_{1at.\%}$ & $\Delta\sigma_{max}$) of the contribution in the yield stress by solid solution strengthening and the reported values ($\Delta\sigma/\Delta c$) by the experiment.

Solute Atoms	Li	Mg	Ag	Mn	Cu	Zn	Ge	Fe
$\Delta\sigma_{1at.\%}$ (MPa)	15.9	25.2	3.1	173.5	51.9	6.3	3.1	205.9
$\Delta\sigma_{max}$ (MPa)	59	109	15	137	82	51	4	36
$\Delta\sigma/\Delta c$ (MPa/at.%)	6.4	30.6	8.0	47.1	45.9	4.1	8.1	446*

$\Delta\sigma_{1at.\%}$; the calculated increment in yield stress when the solute concentration is 1 at%.
$\Delta\sigma_{max}$; the calculated increment in yield stress at the solute concentration of the maximum solid solubility limit.
$\Delta\sigma/\Delta c$; the increment in yield stress by the experiment reported previously when the solute concentration is 1 at%.
* ; the value for Al-1.2 at% Fe alloy.

The prediction from the first-principles calculations, indicating that the misfit strain of the iron atom in aluminum is 3.90 %, suggests that iron is one of the more effective elements to increase its strength in aluminum with less grain boundary embrittlement if the low solid solubility limit in aluminum is not considered. It was previously reported that the vapor quench processed Al-1~3 at% Fe alloys exhibited the high values in yield stress more than about 700 MPa with a reasonable ductility [23]. The ^{57}Fe Mössbauer spectra analyses on a splat quenched Al-1 at% Fe alloy showed that a fraction of the isolated iron atoms (monomer) was about 89 % and that the remaining iron atoms formed the atomic clusters such as dimer (~10 %) and trimer (<1 %) [24]. Also it was pointed out that Al-Fe supersaturated solid solution alloys fabricated by vapor quenching possibly contained the iron atomic clusters, as shown in Fig. 3 [23]. The charge density distribution of the iron monomer and the iron dimer in Al-1.0 at% Fe alloy, as shown in Fig. 4, suggests that the value of the misfit strain for the dimer is higher at -11.1 % in maximum than that for the monomer at -3.9 %. Assuming the mixture rule that the solid solution strengthening due to the iron monomer and the iron dimer is independent each other, Eq. (1) is modified as follows

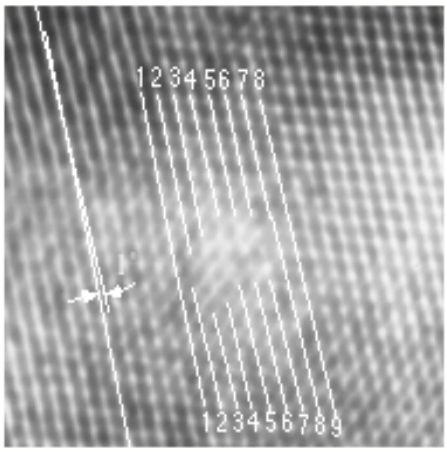

Fig.3 Atomic clusters observed in the Al-Fe supersaturated solid solution alloys fabricated by vapor quenching [23].

$$\Delta\sigma_s = M\frac{3^{3/4}}{2}\left(\frac{1+\nu}{1-\nu}\right)^{3/2}\mu\left(\left|\varepsilon_{\text{monomer}}\right|^{3/2}\sqrt{c_{\text{monomer}}}+\left|\varepsilon_{\text{dimer}}\right|^{3/2}\sqrt{\frac{c_{\text{dimer}}}{2}}\right) \tag{2}$$

where $\varepsilon_{monomer}$ and ε_{dimer} are the misfit strain for the iron monomer and the iron dimer, and $c_{monomer}$ and c_{dimer} are the concentration for the iron monomer and the iron dimer respectively.

In the case of Al-Fe supersaturated solid solution, taking $M = 3.06$, $\mu = 26.5$ GPa [25], $\nu = 0.347$ [25], and $\varepsilon = 0.0390$ which was calculated from the first principles, finally Eq. (2) gives the contribution to the yield stress due to the solid solution strengthening. The dependence of the contribution to the yield stress due to the solid solution strengthening as a function of the iron content is shown in Fig. 5 for a ratio of the dimer concentration to the whole concentration (c_{dimer}/c), including the analytical results obtained using the grain size and the yield stress measured by experimental. The values of $\Delta\sigma_s$ by the analyses from the reported experimental data for Al-1~2 at% Fe alloys are twice or more higher than that of the theoretical values when no existence of the iron dimer is considered. On the other hand, the theoretical values of $\Delta\sigma_s$ when c_{dimer}/c = 0.1~0.2 agree with the experimental data very well. Also these values from 0.1 to 0.2 are corresponding to the fraction of the dimer reported from the Mössbauer spectra analyses for Al-1~2 at% Fe alloys [24].

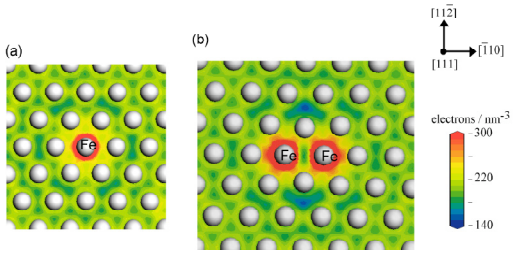

Fig.4 The charge density distribution of the iron monomer and the iron dimer in Al-1.0 at% Fe alloy.

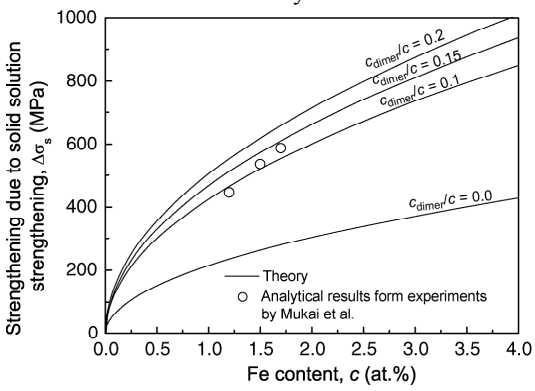

Fig.5 The change of $\Delta\sigma_s$ with c_{dimer}/c estimated from the misfit strain by the first-principles calculations as s function of the iron content; including the experimental data reported [23].

5. Macro-Scaled Fracture Mechanisms

Nanocrystalline Al-Fe alloys with iron content from 1.15 to 1.71 at% were produced by a vapor quenching and were supersaturated solid solution without any identifiable iron-bearing participles, then exhibited a nano-scaled grain size of typically smaller than 100 nm with high-angle grain boundaries, as shown in Fig. 6 [23]. Nominal stress-strain relations of Al-Fe alloys at a strain rate of 10^3 s^{-1} are shown in Fig. 7. Note that the values in flow stress of the present Al-Fe alloys are higher than those of the conventional aluminum alloys with micro order grain sizes, and that the flow stress increases with increasing iron content. An abnormally high tensile strength of ~900 MPa and ductility of about 5% in tension can be obtained in Al-1.7 at% Fe alloy. This indicates that Al-Fe solid solution exhibits the high yield strength with good ductility.

An examination of the fractured specimen revealed that the final fracture event occurred at a macroscopic shear plane inclined more than 45° with respect to the tensile axis, indicating the formation of localized shear bands (Fig.8). The specimen also exhibited a macroscopic necking near the fracture surface, especially in the plate thickness direction. The fracture surface of Al-1.7Fe alloy is shown in Fig. 9. The dimple sizes are also found to be 5 to 10 times the sub-grain size of the present alloys. These images clearly indicate that the local failure process during fracture is ductile in the nanocrystalline Al-Fe alloys, with the mechanism of failure arising from the nucleation, growth and coalescence of voids.

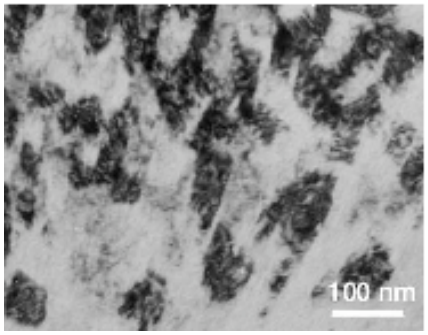

Fig.6 A typical microstructure of nano-crystalline Al-1.2 at% Fe alloy with grains of typically smaller than 100 nm in size.

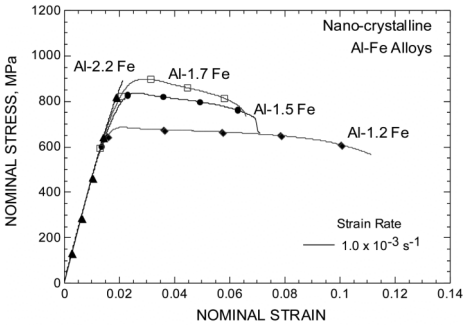

Fig.7 Nominal stress-strain relations of Al-Fe alloys at 10^3 s^{-1}.

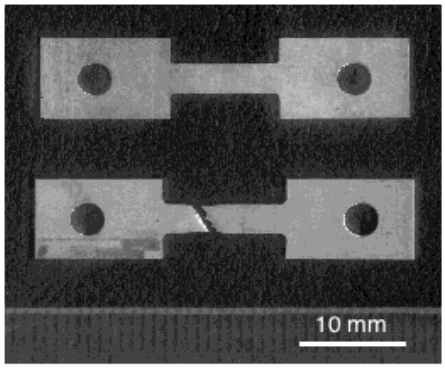

Fig.8 A macroscopic shear plane inclined more than 45° with respect to the tensile axis, indicating the formation of localized shear bands.

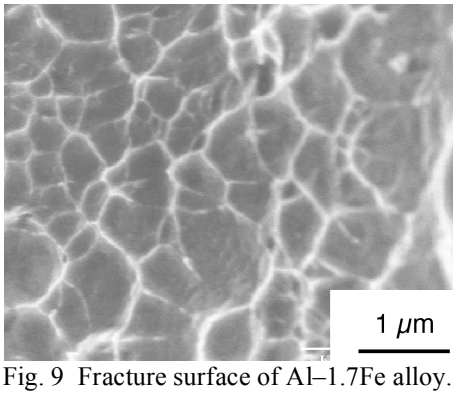

Fig. 9 Fracture surface of Al–1.7Fe alloy.

6. Summary

The solid solution strengthening and the fracture mechanisms of the aluminum alloys were investigated from the multi-length scales analyses, *i.e.*, micro/nano, meso and macro scales researches. As first, the misfit strain, the grain boundary segregation energy and the surface segregation energy in the aluminum binary alloys with 55 solute atoms were calculated from the first principles to identify the more effective strengthen elements with less grain boundary embrittlement such as an intergranular fracture. The calculated results indicated that iron monomer and dimer could create the larger misfit strains at -3.90 and -11.1 respectively in aluminum solution, and the fracture criteria proposed by Rice and Wang subtracted the surface segregation energy from the grain boundary segregation energy of solute atom in aluminum suggested that iron was one of the best

elements to increase its strength in aluminum without grain boundary embrittlement from the knowledge of the atomistic level and the requirement from the element strategy. Al-1.7 at% Fe alloy in supersaturated solid solution produced by a vapor quenching showed an abnormally high tensile strength of ~900 MPa and a relatively good ductility of about 5 % in tension, so it indicates that Al-Fe supersaturated solid solution exhibits the very high strength with good ductility. The analyses using both the misfit strain and the volume fraction of iron monomer or dimer suggested that an unexpected increment in strength results originating in the existence of a fraction of about 20 % of the iron dimer and the rest of the iron monomer. It is postulated that both the nano-grained structures less than 100 nm and the solid solution strengthening due to the large misfit strain by iron solution in aluminum could achieve the abnormal high yield strength of Al-Fe supersaturated solid solution produced by the vapor quenching process.

The contribution to an increment of the yield strength due to the solid solution strengthening could be estimated from the misfit strain. The strengthening mechanisms for the Al-Fe supersaturated solid solution have seldom been discussed from the knowledge of the atomic structure and bonding state. However this analyses from atomistic level by prediction from the first-principles calculations could provide us physical image of the strengthening mechanisms.

Acknowledgements;
Special thanks are due to Dr. T.Uesugi in my laboratory for his help the first-principles calculations.

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