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Aluminum Alloy Chemistry-Microstructure Design and Realization with Modeling

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ABSTRACT The purpose of this paper is to review the art of state of aluminum alloy design, emphasizes are laid on performance-properties, properties-microstructure and chemistry-processing-microstructure relationships. The importance of data bases associated to the alloy design is addressed. The real possibility of aluminum alloy design is evaluated.

Keywords: *Alloy design, model, microstructure-properties relationship, Chemistry-processing-microstructure relationship*

1. INTRODUCTION

Materials design is frequently mentioned as one of the key research and development fields in materials and high technology community. The hope for materials design has been around for some time. As examples, Tien and Ansell have edited a monogram on alloy and microstructure design in 1976 [1], Cocke and Clearfield have organized a symposium on Design of new Materials in 1986 [2].

Aluminum alloys are widely used materials. Experience has been accumulated and the database has been built up from the long-time production and application of aluminum alloys. We have already had more theoretical understandings of fundamental phenomena and underlined mechanisms in aluminum alloy system than that in most other alloy systems. We have already had learnt to control microstructure by processes. We have had many sophisticated experimental means to observe nano/microstructure and measure properties. We have developed some simulation tests for performance of components. Besides, many micro-mechanical models and processing models have been developed for aluminum alloys. Therefore, a quite sound base for aluminum alloy design may be available now [3-27].

Aluminum alloy design project has long been carried out at Alcoa. In Alcoa technical center, they have built a thermo-mechanical processing simulator for processing and microstructure control research and a software to simulate the desired alloy's properties for customers. Pechiney's alloy simulator has been developed for more than 10 years and already been used for alloy developing [25,27], Besides, many research groups and individuals are working on aluminum alloy design, and significant progress is already made [5-8,15-17,19,20,26].

It is worthwhile to review and evaluate the real possibility of aluminum alloy design now.

2. MATERIALS DESIGN

Design is the intellectual attempt to meet certain demands, it is the preparation (invention) of a plan (or a sketch or model etc.) before undertaking the project in order to arrive at the required end-product. It could be qualitative or quantitative, or semi-quantitative.

The term " materials design " is used very loosely in the literatures. It can be used in a broad and a narrow sense. We define defined it as follows:

Materials design is, based on scientific principles, to choose the chemistry and processing and to tailor the microscopic structure and properties of the desired material for a specific performance (application) before actually attempting to make them in the laboratory or plant.

Procedures of Materials Design:

(1) To define the goal and target for the specific application.

First of all, we have to define the goal and object of the desired materials. It is the performance of the material for particular purposes, which is directly related to application.

What is "performance"? It is the "behavior" of the component made of the material. Performance is not simply material's property. There is an ill-defined grey area of expectation between properties of materials and what is achieved in final product performance. In simple situations, we know what properties the material should have to provide the component made of the material the given performance. However, in complicated situations, it is usually difficult or even impossible to predict the performance of the component of the material from the properties of the materials. Different kinds of simulated tests for materials (more and more complicated) have been designed for this purpose. Sometimes they are successful, sometimes not. The most reliable tests are the simulated component tests or even the "trial run" of the machine. Of course the simulated tests and the "trial run" both are very costly.

(2) To build the necessary data base.

In order to build the necessary data base, the information should be collected by searching literatures or performing experiments. The available data base is the foundation of materials design. Missing data should be obtained via direct experimentation or must be predicted via semiempirical or theoretical models.

(3) To collect scientific principles

Theoretical understandings of fundamental phenomena and underlined mechanisms are the vehicles of materials design.

The submodels for the relationships of performance-properties, of microstructure-properties and of chemistry-processing-microstructure should be established.

(4) To choose the material chemistry and processing

Choosing material chemistry and processing and tailoring microscopic structure and properties to meet the goal.

(5) To realize the design by modeling

Modeling the material system with involved submodels. Successful modeling will provide the framework for prescribing the material's properties and performance.

(6) To evaluate the properties and performance by experiments

The evaluation could be either with actual experiments or with computer experiments. The latter eventually should be judged by actual experiments, but it will save much time and money. According to the results of the evaluation, the cycle of material design can be concluded or a new cycle will be started.

3. ALUMINUM ALLOY DESIGN

The development of aluminum alloy mill products for the aerospace industry, according to James Staley [4], may consists of the following stages :

Perform research to develop new knowledge.
Identify opportunity for new materials.
Establish tentative property goals and alternative approaches.
Develop preliminary business plan.
Perform laboratory processing and testing.
Establish firm target properties.
Verify with plant trial.

Obtain customer feedback.
Establish guaranteed properties.
Confirm that plant can meet all guarantees.
Develop detailed business plan.
Implement commercially.

The first few stages are involved in the alloy design.

The following flow chart is taken as the logical sequence for aluminum alloy design, Fig. 1.

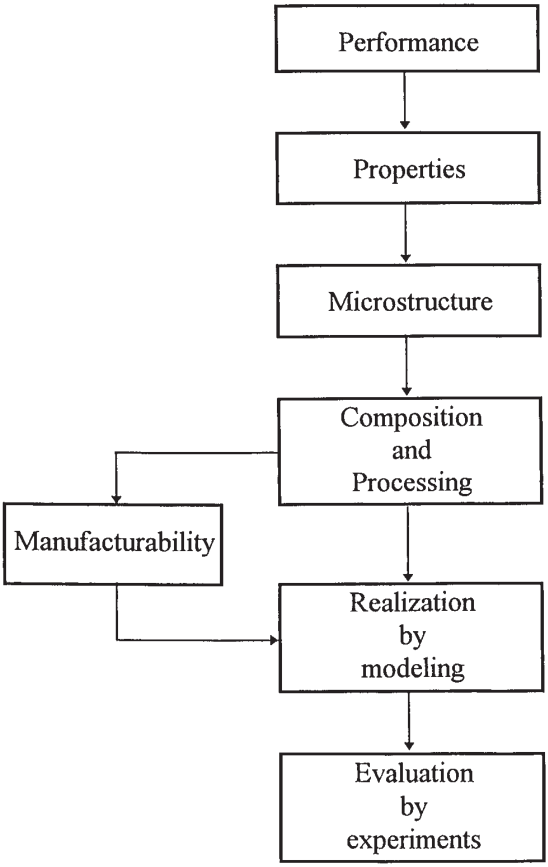

Fig. 1 Logical sequence of alloy design

3.1 Performance

The performance of the alloy for particular application has to be defined at first. It is the "behavior" of the component made of the desired alloy. The performance of the alloy for the fuel tank of space shutter, for ships, for beverage cans, for the plate armor, are very different. It is not always possible to predict the requirement of alloy's properties for the desired performance. Therefore, the simulated tests are necessary in some cases.

3.2 Properties

Physical, chemical and mechanical properties are direct requirements for the desired material being designed.

The most common required properties for aluminum alloys are: density, coefficient of expansion, specific heat, electrical conductivity, UTS, YTS, elongation, Young's modules, Poison's ratio, hardness, general corrosion resistance. Further requirement may be: K_{IC}, K_C, S-N curves, da/dt, LCF, EXCO resistance, SCC resistance, low temperature strength, high temperature strength, creep resistance, wear etc.

We have to make best use of our understanding to predict which properties of the designed alloy should have to provide the desired performance of the component. For example, the performance of the alloy for the low temperature fuel tank of the aerospace industry may involve high strength at low temperature, low temperature ductility, low temperature toughness and good weldability etc. The relationships between performance and properties are the vehicles for this purpose. Only in simple situations, we have enough knowledge to predict properties for the desired performance. In complicated situations, we can not predict properties for the desired performance. For instance, the spectrum loading fatigue resistance, multi-axial fatigue and toughness, fatigue-creep-environment interrelationship etc.

There are interrelations among properties, to improve some properties usually have to sacrifice in other properties. You have to keep balance among properties for specific purpose. It is well known that the increasing of strength of a material will hurt its ductility and toughness.

3.3 Microstructure

The relationships between microstructure and properties are used to predict the desired microstructure for the designed materials. We have much better understanding for microstructure-properties relationships than that for properties-performance relationships [7,9-15,17,18,21,23].

Microstructure properties relationships and associated data bases are listed in Table 1.

3.4 Composition and processing

The relationships among alloy chemistry, processing and microstructure are used to predict the desired composition and processing for the desired microstructure [5,6,8,19,20,22,24,25,26,28,29]. They provide the ability to model the influence of changes in alloy chemistry and processing route to optimize the microstructure.

The relationships of composition-processing-microstructure and associated data bases are listed in Table 2.

3.5 Manufacturability

The manufacturability is very important for the application of the alloy.

The relationships of manufacturability-chemistry-microstructure are used to design the chemistry and microstructure of the alloy for the desired manufacturability [6,19,26].

The relationships of manufacturability-chemistry-microstructure and associated data bases are listed in Table 3.

Table 1 Microstructure - properties relationships

Submodels	Data base
Strength: Solid solution strengthening Strain strengthening Precipitation strengthening Grain size strengthening Substructure strengthening Ductility: cleavage, ductile and intergranular shear failure Toughness: intrinsic toughening extrinsic toughening Fatigue: crack initiation crack propagation: Paris law HCF: S-N curves LCF: Manson-Coffin law etc. Corrosion: pitting exfoliation stress-corrosion cracking (SCC)	matrix: nature and properties crystal plasticity grain structure: size, shape, orientation grain boundary: properties, segregation, second phase textures Second-phase particles: Stable or metastable Precipitates: nature, properties, size, shape, density, distribution dispersoids: nature, properties, size, shape, density, distribution inclusions: nature, properties, size, shape, density, distribution Interface: coherency and misfit: coherent, semi-coherent or incoherent precipitate-free zone (PFZ) segregation

Table 2 Chemistry - processing - microstructure relationships

Submodel	data base
Constitution - microstructure submodel thermodynamics and phase diagram diffusion mechanisms phase transformation - microstructure equilibrium and nonequilibrium solidification - microstructure rapid solidification - microstructure **Processing - microstructure submodel** cold and hot working - microstructure solution treatment and rapid cooling nucleation, growth and coarsening of precipitates thermo-mechanical process - microstructure powder metallurgy: pressing and sintering, HIP and heat treatment novel process techniques	thermodynamics data equilibrium diagram diffusion coefficient and mechanisms phase transformation data kinetics and activation energy crystal structure and defects precipitation sequence second-phase particles: nature, size, shape, density and distribution trace element effects hydrogen effect

Table 3 Manufacturability - chemistry - microstructure relationship

Submodel	data base
Workability Formability Superplasticity Castability Weldability	stress -strain curves flow stress data process variables effects specific heat heat conductivity coefficient of expansion viscosity surface tension

3.6 Realization by modeling

Modeling the designed alloy with involved submodels will provide the framework for prescribing the material's properties and performance [5,6,8,16,19].

3.7 Evaluate the model by experiments

The evaluation could be with either actual experiments or computer experiments. According to the results of the evaluation, the alloy design cycle can be concluded or a new design cycle will be started, Fig.2.

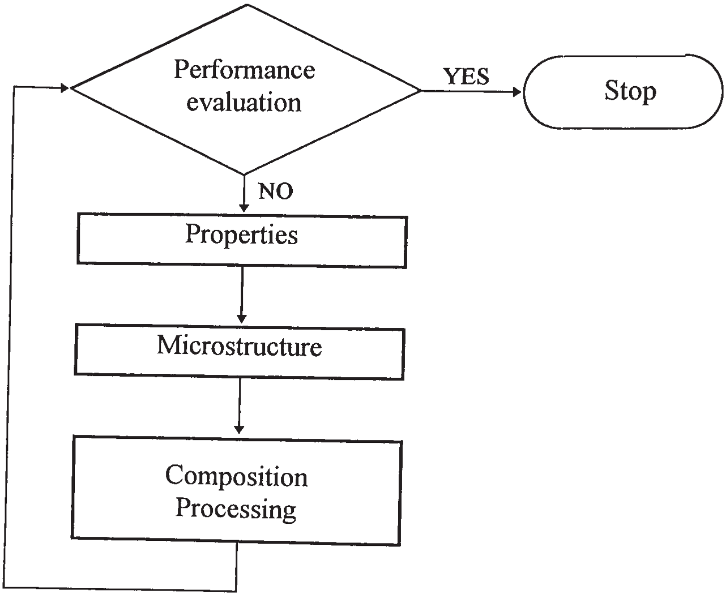

Fig.2 Alloy design cycle

An single alloy designed fully by logical way as described in this paper has not been found till now. But there are a few alloys designed more or less deliberately. The aluminum-lithium alloy Weldalite 049, then 2097, Alcoa's 7055-T77 for upper wing of Boeing 777, Pechney's new upper wing alloy 7349 and 7449 etc.

4. SUMMARY

The necessary submodels and data base for a complete materials design, even only for aluminum alloy system are enormously large. No single individual could manage all the problems involved in the alloy design. A system engineer is necessary to work together with a group of experts in many different disciplines for this enormous undertaking task. It is usually needed to fill important gaps in understanding and to develop theories that provide quantitative guidelines for the design of materials, and to collect associated data by experiments.

The long-term nature of materials design and the relatively short turn-around time for trial and error approaches have limited industrial attempts. The materials generally are not designed for the application but rather are selected and modified for the application.

It is still a quite long way to make the process of aluminum alloy design a real routine.

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REFERENCES

[1] J.K. Tien and G.S. Ansell, Alloy and Microstructural Design, Academic Press, N.Y., (1976).
[2] D.L. Cocke, Design of New Materials, D.L. Cocke and A. Clearfield eds., Plenum Press, New York, (1987).
[3] J.W. Martin, Micromechnisms in particle-hardened alloys, Cambridge University Press, (1990).
[4] J.T. Staley, ***Indian J. Technology***, **28**, (1990), 226.
[5] H.R. Shercliff and M.F. Ashby, ***Acta Metall. Mater.***, **38**, (1990), 1789.
[6] O.R. Myhr and Ø. Grong, ***Acta Metall. Mater.***, **39**, (1991), 2693.
[7] E. Hornbogen and E.A. Starke,Jr., ***Acta Metall. Mater.***, **41**, (1993), 1.
[8] D.H. Bratland et al, ***Acta Metar.*** **45**, (1997), 1.
[9] C.Q. Chen and J.F. Knott, ***Metal Science***, **15**, (1981), 357.
[10] C.Q. Chen and H.X. Li, ***Mater. Sci. Tech.***, **3**, (1987), 125.
[11] G.B. Zhang and C.Q. Chen, ***Acta Met. Sinica*** (English Edition), **3A**, No.4, (1990), 262.
[12] C.Q. Chen and H.X. Li, ***Mater. Sci. Tech.***, **6**, (1990), 850.
[13] C.Q. Chen, Science and Engineering of Light Metals, eds. K.Hirano, JILM, (1991), 185.
[14] J.T. Staley, Proc. ICAA3, L. Arnberg et al eds., Trondheim, (1992), 107.
[15] G.M. Raynaud, B. Grange and C. Sigli, Proc. ICAA3, L. Arnberg et al eds., Trondheim, (1992), 169.
[16] R.D. Doherty, Proc. ICAA3, L. Arnberg et al eds., Trondheim, (1992), 261.
[17] E.A. Starke,Jr., E. Hornbogen and C.P. Blankenship,Jr., Proc. ICAA3, L. Arnberg et al eds., Trondheim, (1992), 279.
[18] J.F. Knott, Proc. ICAA3, L. Arnberg et al eds., Trondheim, (1992), 215.
[19] C.M. Sellars, Proc. ICAA3, L. Arnberg et al eds., Trondheim, (1992), 89.
[20] H.R. Shercliff et al, Proc. ICAA3, L. Arnberg et al eds., Trondheim, (1992), 357.
[21] K. Nisancioglu, Proc. ICAA3, L. Arnberg et al eds., Trondheim, (1992), 239.
[22] G.J. Marshall, ***Mater. Sci. Forum***, **217-222**, (1996), 19.
[23] J.D. Embury, ***Mater. Sci. Forum***, **217-222**, (1996), 57.

[24] N. Saunders, ***Mater. Sci. Forum***, **217-222**, (1996), 667.
[25] C. Sigli, H. Vichery and B. Grange, ***Mater. Sci. Forum***, **217-222**, (1996), 391.
[26] ∅ystein Grong, ***Mater. Sci. Forum***, **217-222**, (1996), 107.
[27] P. Sainfort et al., ***Mater. Sci. Forum***, **242**, (1997), 25.
[28] B.C. Wei et al, in this Proceedings.
[29] R. Chen et al, in this Proceedings.