The Metallurgical Database of Aladin
-an Alloy Design System

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Table of Contents

List of Figures

Abstract

Aladin is an expert system that aids metallurgists in the design of new aluminum alloys. Declarative structured representations in the form of schemata are used for metallurgical data and concepts. The representation is very general, the goal has been to create a representation for all knowledge about aluminum alloys and metallurgy relevant to the design process. This article gives an overview of the alloy database and describes the architecture of the microstructure database in detail. The microstructure of alloys is described by an enumeration of the types of microstructural elements present along with their characteristics.

1 Introduction

The metallurgical knowledge base of Aladin is created to form a knowledge medium for metallurgical knowledge with the goal to fill the needs of the design task, i.e. representing all knowledge needed to design an alloy. Alloy design is a knowledge-intensive enterprise, the knowledge representation must therefore handle a broad range of different kinds of knowledge. If the alloy design process is viewed as a mapping from functional description to a production process description the need for representations of physical properties, chemical composition and thermomechanical process operations emerges immediately. Furthermore, the science of metallurgy identifies understanding of the microstructure as a powerful tool to reason about alloy design, which introduces the need for a representation of microstructural features and phase diagrams. In general all models that are used to reason about alloy design and all concepts that they deal with need to be represented.

In the design of new alloys, researchers depend heavily on their understanding of existing alloy systems, standard production methods, and the observed effects of composition, treatments and structural variations on key properties. The amount of knowledge required to successfully develop new materials is so great that individuals often can not complete the task alone. They must supplement their private knowledge with information obtained from text books, journal articles and highly specialized consultants. ALADIN is designed to contain a detailed and extensive knowledge bank of metallurgical information. This bank will serve as a reference manual for designers that have specific questions about alloy characteristics, microstructures, phases, production methods and applications. The knowledge bank is also accessed by ALADIN's inference procedures when researchers ask for suggestions about various design tasks.

ALADIN utilizes three forms of knowledge representations:

1. **Declarative** knowledge base of alloys, properties, products, processes, and metallurgical structure concepts;

2. **Production Rules** in the form of IF-THEN rules of many types: control of search among competing hypotheses, empirical associations of causes and effects, rankings and preference orderings, decisions about when to call upon knowledge in other forms, and others;

3. **Algorithmic** knowledge expressed as functions: detailed physical, statistical and other procedural computations.

In this paper, the knowledge medium created by the declarative knowledge representation of the ALADIN system will be discussed with emphasis on microstructure representations. For descriptions of other aspects as well as an overview of the system see the references [8, 4, 10, 3, 9].

The declarative knowledge is structured through the use of hierarchies of schemata. The representation has a hierarchy of abstraction levels which contains different degrees of detail. The facilities of Knowledge Craft [13, 2] are utilized to define relationships and inheritance semantics (see [2]) between metallurgical concepts [5]. The most commonly used relations are IS-A and INSTANCE. The IS-A relation defines hierarchies of classes or groups where each higher level subsumes the lower level classes. The INSTANCE relation declares a particular object to belong to a class or a group and the description of the class serves as a prototype of the instances. The knowledge bank contains information about alloys, products and applications, composition, physical properties, process methods, microstructure and phase diagrams. The representation is very general, the goal has been to create a representation for all knowledge about aluminum alloys and metallurgy relevant to the design process. Our involvement with aluminum alloys and with experts on aluminum has introduced a bias towards aluminum and its alloys but we are convinced that the framework of the knowledge representation is useful for other alloy families and to some extent even for other materials. The representation of alloys is representative of most of the database and will therefore be discussed in some detail, followed by a discussion on microstructure which requires a more involved representation.

2 Alloys

Alloys, when viewed from the standpoint of their design, are interrelated and grouped in a number of different ways. We have defined a number of relationships, with different inheritance semantics, to enable our schemata to reflect this domain organization. For example, alloys are grouped together into series and families by their
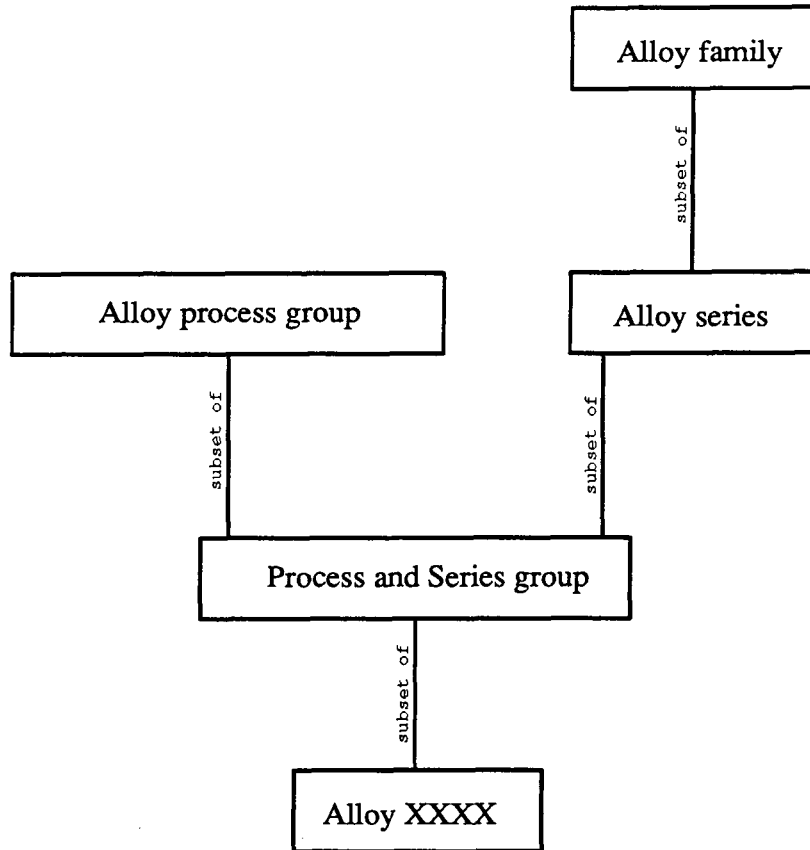
```
                                          ┌─────────────────┐
                                          │   Alloy family  │
                                          └─────────────────┘
                                                   │
                                                subset of
                                                   │
┌─────────────────────────┐          ┌─────────────────┐
│   Alloy process group   │          │   Alloy series  │
└─────────────────────────┘          └─────────────────┘
            │                                 │
         subset of                         subset of
            │                                 │
         ┌─────────────────────────────────────┐
         │       Process and Series group      │
         └─────────────────────────────────────┘
                          │
                       subset of
                          │
                   ┌─────────────────┐
                   │   Alloy XXXX    │
                   └─────────────────┘
```

Figure 1: Alloy Groups

composition. They are also related by the processes that go into their fabrication (e.g., heat treatment, cold rolling, and tempering), by the type of application that an alloy is designed for, and by the form of product (e.g., sheet, plate, or extrusion). Relations have been defined to reflect degrees of abstraction within the hierarchy, e.g., the relationship between a family and a prototypical member. These relations are used at various stages in the design search in order to make hypotheses and estimates. By defining classes of similar alloys they allow analogies to be drawn along a number of different dimensions. Figure 1 depicts some of this knowledge-base structure. Schemata are used to define all of the relations and abstract entities involved.

The classification of alloys into series and process groups is useful, for example, to look for trends. These trends can be used to derive design options (the addition of elements, the specification of processing parameters, etc.) that are likely to produce an alloy with desired properties. When searching for trends, however, care must be taken to look for alloys that are produced in similar ways, have similar compositions, and were tested using identical methods. Some of these restrictions may be imposed by comparing only alloys from the same alloy-process-group and/or alloy-series.

We will use the 2024-T8-sheet alloy, as defined in references [6] and [1] to illustrate the knowledge representation. In the ALADIN data base, five schemata, shown in figures 2 - 6, are required to describe this alloy.

The following information is represented in figure 2: The alloy is a member of the 2xxx-T8-sheet group of alloys which is further defined in the schema shown in figure 3. The application of this alloy is aerospace. Several properties such as elongation have known values and they are given. The major and minor alloying elements as well as impurity elements along with their respective nominal percentages are specified. The microstructure is described by a schema in figure 6.

```
{{ 2024-T8-sheet
        INSTANCE: alloy
        MEMBER-OF: 2xxx-T8-sheet
        ELONGATION: 6
        ...
        APPLICATION: aerospace
        ADDITIVES:
                Cu
                        nominal-percent: 4.4
                        class: major-alloying-element
                        unit: weight-percent
                Mg
                        nominal-percent: 1.5
                        class: major-alloying-element
                        unit: weight-percent
                Mn ...
                Fe ...
                Si ...
        MICROSTRUCTURE: 2024-T8-sheet-strct
                }}
```

Figure 2: The 2024 Alloy

```
{{ 2xxx-T8-sheet
        INSTANCE: process&series-group
        SUBSET-OF: 2xxx-series-2 sheet-group T8-temper-group
        ELONGATION: 7
        MODULUS: 10.6
        ...
        MACHINABILITY: B
        TENSILE-YIELD-STRESS:
                range: (pred (lambda (x) (and (> x 51) (< x 66) ) ))
        FATIGUE:
                linguistic: (or low medium)
        }}
```

Figure 3: The 2-Thousand Series and Process Group

The process and series group shown in figure 3 is associated with the following information: It is a subset of the 2xxx-series, the sheet-group and the T8-temper-group. The sheet-group and the T8-temper-group schemata are shown in figures 4 and 5. Information on several properties is given. Explicit property values serves as default values for members of the group, eg. if the 2024-T8-sheet schema lacks information on modulus the modulus value of 2xxx-T8-sheet will be used. At the same time, the more specific elongation value of 2024-T8-sheet overrides the value of 2xxx-T8-sheet. The expression in the range attribute of a property is a constraint on possible values of that property for members of the group. This constraint is coded in lisp and in this case it means that the tensile yield stress is between 51 and 66 ksi. Aladin also uses linguistic variables to define ranges of values and here the fatigue is constrained to be low to medium. The meanings of linguistic variables are defined in the property database.

```
{{ sheet-group
        INSTANCE: alloy-process-group
        PRODUCT: sheet
        PROCESS-METHODS: cast preheat hot-roll
                cold-roll }}
```

Figure 4: The Sheet Process Group

The sheet-group schema, figure 4, provides information that is common for sheet products, namely a specific sequence of process methods that is used to make sheet aluminum.

```
{{ T8-temper-group
        INSTANCE: alloy-process-group
        TEMPER: T8
        PROCESS-METHODS:
                solution-heat-treat ...
                quench ...
                stretch  ...
                age
                        type-of: age
                        level: peak
                        class: artificial  }}
```

Figure 5: The T8-Temper

The T8-temper-group schema, figure 5, specifies the process methods that determine the temper of the alloy.

Finally, the 2024-T8-sheet-strc schema shown in figure 6 gives information about the microstructure. This alloy is a multi-phase dispersion. Rod shaped S prime precipitates, 0.1 micron in size, are distributed uniformly throughout the metal. The alloy is fully recrystallized with elongated grains of 40 microns in size. The microstructure representation is described in detail in section 3 and an example from the metallurgical research literature is examined in 3.3.

```
{{ 2024-T8-sheet-strct
        INSTANCE: multi-phase-dispersion
        STRUCTURE-ELEMENTS:
            grain
                instance: microstructural-element
                size: 40
                recrystallization-level:
                        recrystallized
                                instance: value
                                %: 100
                aspect-ratio: 2
                texture: cube
            precipitate
                instance: microstructural-element
                phase: s-prime
                size: 0.1
                aspect-ratio: 100
                geometry: rod
                distribution: uniform
        .....}}
```

Figure 6: The 2024 Microstructure Representation

3 Microstructure

The term "microstructure" will here be used for alloy features between the levels of crystal structure and macroscopic structures exclusively, while the word "structure" includes both microstructure and phases. Ideally a pure solid solution would form a perfect single crystal, but in practice nonequilibrium phenomena and insoluble phases introduces structural features. Hence, microstructure can be defined to be the configuration in three dimensional space of all types of non-equilibrium defects [7]. Metallurgical research has shown that many microstructural features have important consequences for macroscopical properties. The objective of the microstructure representation in Aladin is to classify and quantify the microstructure of alloys in order to facilitate the application of quantitative and qualitative models that relate the microstructure to the properties of alloys or to processing and composition. The representation of microstructure presents some interesting problems and is discussed in detail here.
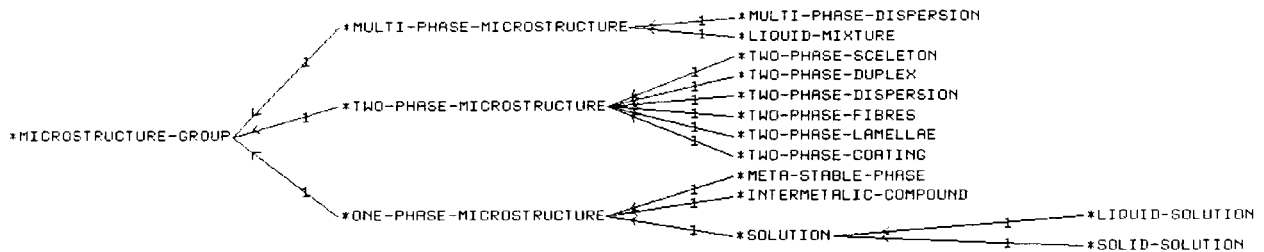
*MICROSTRUCTURE-GROUP
*MULTI-PHASE-MICROSTRUCTURE
*MULTI-PHASE-DISPERSION
*LIQUID-MIXTURE
*TWO-PHASE-MICROSTRUCTURE
*TWO-PHASE-SCELETON
*TWO-PHASE-DUPLEX
*TWO-PHASE-DISPERSION
*TWO-PHASE-FIBRES
*TWO-PHASE-LAMELLAE
*TWO-PHASE-COATING
*ONE-PHASE-MICROSTRUCTURE
*META-STABLE-PHASE
*INTERMETALIC-COMPOUND
*SOLUTION
*LIQUID-SOLUTION
*SOLID-SOLUTION

Figure 7: Classification of Microstructure

Although much of the heuristic knowledge about alloy design involves the microstructure it is usually poorly represented. Metallurgists have attempted to describe microstructural features systematically [7] and there is also a field called quantitative metallography that describes quantitative information about the three-dimensional microstructure of alloys [11], in practice neither approach is commonly used. Instead metallurgists rely on visual inspection of micrographs, pictures of metal surfaces taken using a microscope. Information is communicated with these pictures and through a verbal explanation of their essential features.

The reasons why metallurgists prefer linguistic rather than quantitative descriptions of the microstructure lies in the adequacy of the former. In many practical applications the source of poor performance of an alloy can be attributed to the presence or absence of certain microstructural features, without necessity of knowing all their characteristics. For example, high yield strength is often achieved by drastically reducing grain size through suppression of recrystallization. Since the difference between recrystallized and unrecrystallized structures are apparent, one glance at the micrograph can tell metallurgists if the improvement of yield strength is feasible by this method. If grains are several hundred microns in diameter, e.g. "large" in metallurgical nomenclature, the structure is recrystallized and suppression of recrystallization is a valuable option to improve strength. When grains are "small", e.g. only several microns in diameter, the structure is unrecrystallized and some other methods of strength improvement will have to be used. Presence or absence of precipitates, precipitation free zones, particles, voids etc. are other indicators used by metallurgists for qualitative description of the microstructure.

There is also a human aspect to the preferential use of qualitative descriptions. Determination of any of the quantitative descriptors of the microstructure requires hundreds of repetitious measurements. In the past these measurements had to be made by hand hence they were too time consuming to be used in everyday practice. Recent developments in image processing techniques made automation of these methods possible and we expect wider use of the quantitative description of microstructure by metallurgists in the future.

In order to represent microstructure data and rules it was necessary to develop a symbolic representation of alloy microstructure. Microstructures are classified as described by Hornbogen [7] and shown in Figure 7. The two main features of an alloy microstructure are the grains and the grain boundaries. The microstructure is described by an enumeration of the types of grains and grain boundaries present. Each of these microstructural elements is in turn described by any available information such as size, distribution etc. Each of these elements can also be associated with other microstructural elements such as precipitates, dislocations etc. This representation allows important facts to be expressed even if quantitative data is unavailable. An important example is the presence of precipitates on the grain boundaries. It is interesting to note that most of the expert reasoning about microstructure deals with qualitative facts and that quantitative information is typically not available.
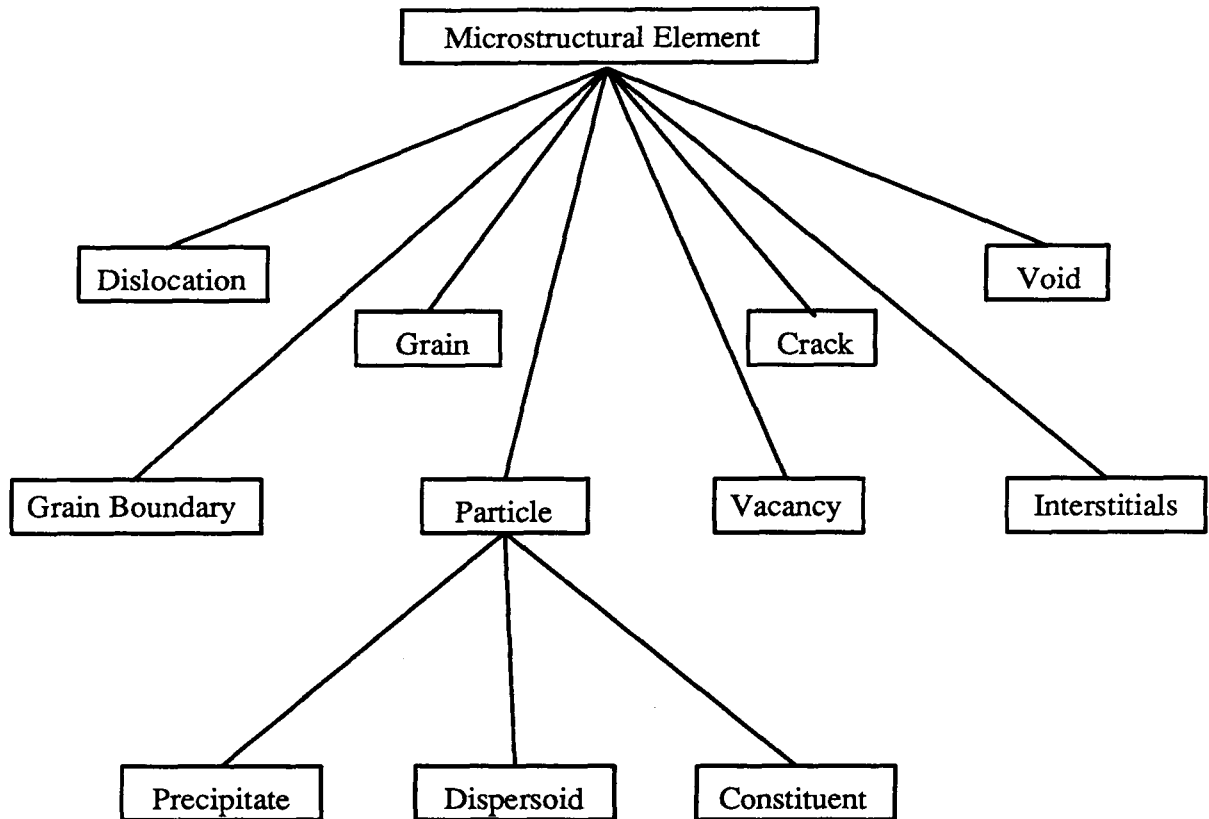
Figure 8: Taxonomy of Microstructural Elements

3.1 Structured Representation of Microstructure

The representation of alloys (figure 1) includes the attribute MICROSTRUCTURE that gives the name of a schema that describes the microstructure. In the case of 2024-T8-sheet (see figures 2 and 17) the microstructure is described in the schema 2024-T8-sheet-strct which is an instance of a multi-phase-dispersion. Microstructures are in general classified in one of the categories shown in figure 7 or some subcategory of them. The ability to create new subcategories makes the representation flexible and extendable to other alloy families. If this representation were to be applied to steel, for example, a martensitic microstructure could be defined and added to the microstructure groups. The schema shown in figure 9 defines the attributes that are associated with a microstructure group and the relation to other concepts (through the IS-A attribute and and its inverse IS-A+INV). The *range* attribute constrains the possible values of an attribute.

{{ **MICROSTRUCTURE-GROUP**
    IS-A: alloy-property
    IS-A+INV: multi-phase-microstructure two-phase-microstructure amorphous-solid one-phase-microstructure
    STRUCTURE-ELEMENTS:
        range: (all (type instance microstructural-element))
    NUMBER-OF-PHASES:
        range: (pred crl-iplusp) }}

Figure 9: The top of the microstructure hierarchy

3.2 Microstructural Elements

The microstructure is further characterized by a description of the microstructural elements that are present. The basic elements of microstructure are shown in figure 8 and the attribute STRUCTURE-ELEMENTS holds an enumeration of such elements. The microstructural elements themselves are schemata related to the schema in figure 10 which again defines what attributes are associated with a microstructural element and some restrictions on their values and the dimensionality of the element.

```
{{ MICROSTRUCTURAL-ELEMENT
    IS-A: concept
    IS-A+INV: crack void particle grain grain-boundary dislocation interstitials vacancy droplet liquid
    FORMATION-MODE:
        range: (or massive-transformation local-transformation)
    ELEMENT-DENSITY:
    DIMENSION:
        range: (or 0 1 2 3)
    STRUCTURE-ELEMENTS:
        range: (all (type instance microstructural-element)) }}
```

Figure 10: Microstructure Element

Figure 8 shows that the Aladin database defines eight types of microstructural elements and additional subclasses. Each of these microstructural elements is further described by attributes such as size, shape, orientation and distribution as described in subsequent paragraphs. This information is attached to the structure-element name appearing as a value of the STRUCTURE-ELEMENT attribute (see figures 6, 18 and 19), this is called a meta value. In general, numeric values for many quantities can be accompanied with meta information or meta values, carrying additional information on the value such as statistical distribution and standard deviation or specification of the method used to obtain the value.

An important feature of this representation is that the attribute STRUCTURE-ELEMENTS may appear again in a schema describing a structure element. This allows representation of structure features with sizes of different order of magnitude. Specifically it provides a means to specify the location of particles such as precipitates, a particle type can belong to one kind of grain or to the grain boundary. The details of the representation of microstructural elements are given in the following paragraphs. The schemata showed in the following paragraphs are representative of the schemata that are attached as meta values to the values of the STRUCTURE-ELEMENT attribute.

Grain. Grains are the largest elements of the microstructure. One or more types of grains can be present depending on whether the type of microstructure is one-phase or not. The schema representing the concept grain is shown in figure 11 and it defines the attributes of a grain. The phase attribute defines what phase the grain belong to. The size attribute gives the average diameter of a grain; for non-spherical grains length, width, etc. can be given as meta values. The aspect-ratio measures the deviation from spherical symmetry and can be augmented with information on alignment of the grains. The texture gives information on effect of mechanical processing versus the degree of recrystallization. The recrystallization-level can also be specified by the RECRYSTALLIZATION-LEVEL attribute independent of the texture. Fracture mode can be transgranular or intergranular. Physical properties such as strength can also be specified.

```
{{ GRAIN
    IS-A: microstructural-element
    PHASE:
        range: (type is-a phase)
    SIZE:
    ASPECT-RATIO:
    TEXTURE:
        range: (all (or copper brass S cube Goss))))
    RECRYSTALLIZATION-LEVEL:
        range: (or recrystallized partial unrecrystallized)
    FRACTURE-MODE:
    STRENGTH: }}
```

Figure 11: Prototypical Grain

Grain Boundary. A description of the grain boundaries are important in many cases and the representation is shown by the grain boundary schema, figure 12. The TYPE of grain boundary describes the relation between the orientation of neighboring grains. The ANGLE is the angle of mismatch in the orientation of crystal lattices. The PFZ-ZONE enumerates precipitates that are depleted around the the grain boundary. The IMPURITY enumerates elements that are enriched at the grain boundary. In addition some physical properties can be associated with a grain boundary.

```
{{ GRAIN-BOUNDARY
     IS-A: microstructural-element
     DIMENSION: 2
     TYPE:
         range: (or tilt twist mixed)
     ANGLE:
         range: (or low medium high)
     PFZ-ZONE:
     IMPURITY:
         range: (type is-a element)
     STRENGTH:
     STRESS: }}
```

Figure 12: Prototypical Grain Boundary

Particle. Particle is the prototype for precipitates, dispersoids and constituents, their representation follows the pattern of the schema in figure 13. The SIZE and ASPECT-RATIO is specified as for grains. The GEOMETRY can be sphere, rod etc. The DISTRIBUTION of the particle can be uniform or clustered etc. The PHASE and VOLUME-FRACTION attributes holds corresponding information and the STABILITY attribute shows whether the particle is stable or meta-stable.

```
{{ PARTICLE
     IS-A: microstructural-element
     IS-A+INV: precipitate dispersoid constituent
     DIMENSION: 3
     SIZE:
     ASPECT-RATIO:
     GEOMETRY:
         range: (or sphere rod plate oblate-sphere)
     DISTRIBUTION:
         range: (or uniform clustered regular)
     PHASE:
         range: (type is-a phase)
     VOLUME-FRACTION:
     STABILITY:
         range: (or equilibrium meta-stable) }}
```

Figure 13: Prototypical Particle

Dislocations. In the dislocation schema, figure 14, the TYPE attribute is similar to the TYPE in grain-boundary. Dislocations can also have ELEMENT-DENSITY and DISTRIBUTION.

```
{{ DISLOCATION
     IS-A: microstructural-element
     TYPE:
         range: (or edge screw mixed)
     DIMENSION: 1 }}
```

Figure 14: Dislocation

Other Structure Elements. The other structure elements are represented by schemata in figure 15, the meaning of attributes follows the pattern described above.

```
{{ CRACK
    IS-A: microstructural-element
    DIMENSION: 2
    LENGTH:
    WIDTH:}}

{{ VOID
    IS-A: microstructural-element
    DIMENSION: 3
    VOLUME-FRACTION:
    SIZE:
    ASPECT-RATIO:
    DISTRIBUTION:
        range: (or uniform clustered regular) }}

{{ INTERSTITIALS
    IS-A: microstructural-element
    DIMENSION: 0 }}

{{ VACANCY
    IS-A: microstructural-element
    DIMENSION: 0 }}
```

Figure 15: Other Structure Elements

3.3 Examples of Microstructure Representation

Two examples of microstructures of Al-3Li-0.5Mn alloys, from Vasudevan et al [12], are shown in figures 16a and 16b. They show the alloy after solution heat treatment and cold water quenching (SHT) and additionally peak aged at 400°F for 48 hours (PA) respectively (see figure 17). The main difference between the alloys is that an alloy in SHT condition has most of the lithium in solid solution while for the one in PA condition most of the lithium is contained in the form of precipitates.

Vasudevan et al describes these microstructres verbaly as follows:

"[16a] shows the as-quenched microstructure of the alloy (condition A with zero aging) where no grain boundary δ is observed although a very fine matrix δ' can be seen as a faint mottling. This δ' was presumably produced during the quench. Figure [16b] shows the microstructure in the peak-aged alloy (condition B), where the strengthening matrix δ' precipitates are seen together with coarse grain boundary δ precipitates; these are seen as white regions surrounded by dislocations ... and a δ' precipitate-free zone (PFZ) 0.5 μm wide which has given up its solute to the grain boundary δ."

The microstructure representations for both alloys, used in ALADIN, are shown in figures 18 and 19. Notice that in the case of SHT alloy it is classified as a two-phase-dispersion rather than solid-solution, as most metallurgists would expect. This is due to the fact that although all lithium is in solid solution after solutionizing treatment, this alloy contains grain size controlling Al_6Mn dispersoids, scattered inside grains, which also give some amount of dispersion strengthening to the alloy. Other characteristics of the microstructure, i.e. that it is recrystallized, has high angle grain boundaries, elongated grains parallel to the rolling direction and low dislocation density are also properly represented. The schema representation is not limited to characteristics that are apparent on a micrograph and includes qantitative information.

In case of PA alloy most of the lithium is in the form of either δ' precipitates inside grains or δ particles on the grain boundary. Grain boundary has additionally precipitation free zone (PFZ) but other characteristics of the microstructure, such as $MnAl_6$ dispersoids, are the same as for the SHT case as they are not affected by the aging treatment. Note that treating grain interior and grain boundary as separate microstructural elements allowed for the association of δ particles and PFZ with the grain boundary, a crucial feature in this microstructure.

It is also important to point out that due to the recursive property of the above representation, i.e. each microstructural element can have any other microstructural element even one of the same class, making it possible

Figure 16: Micrograph of Al-3Li-0.5Mn; a. as Quenched, b. Peak Aged Condition
(from [12])

```
{{ Al-3Li-0.5Mn-pa
   MEMBER-OF: experimentAl-Li-Mn-series
   MICROSTRUCTURE: Al-3Li-0.5Mn-pa-strc
   ADDITIVES:
      Li
         nominal-percent: 3.0
         unit: weight-percent
      Mn
         nominal-percent: 0.5
         unit: weight-percent
   PROCESS-METHODS:
      cast
         class: direct
      solution-heat-treat
         temperature: 1020
         time: 30
      stretch
         percent-stretch: 2
      age
         time: 48
         temperature: 400
         level: peak
         class: artificial }}
```

Figure 17: Representation of Al-3Li-0.5Mn in Peak Aged Condition,
the age process method is omitted in the quenched condition.

to represent any imaginable microstructure. For example let's assume that the solution heat treated alloy has subgrains inside each grain and that each [subgrain consists of several cells separated by dislocation angles. In Aladin, such a structure will be represented as grains with high angle boundaries containing small grains with low

angle boundaries, which in turn have also small grains with low or medium dislocation density of the boundaries. Since grains at each "level" can have variety of microstructural elements, all possible microstructures can be easily represented using this method.

```
{{ Al-3Li-0.5Mn-sht-strc
    MICROSTRUCTURE-FOR: Al-3Li-0.5Mn-sht
    STRUCTURE-ELEMENTS:
        grain
            size:
                length: 415
            aspect-ratio: 4
                alignment: rolling-direction
            texture:
                copper
                    volume-fraction: 0.02
                brass
                    volume-fraction: 0.02
                S
                    volume-fraction: 0.02
                cube
                    volume-fraction: 0.70
                Goss
                    volume-fraction: 0.24
            recrystallization-level: 100
            phase: alpha-Al-Li
            structure-elements:
                dispersoid
                    phase: Al6-Mn
                    size:
                        0.2
                            probability-distribution: log-normal
                    aspect-ratio: 3
                        geometry:
                            rod
                                length: 0.3
                    volume-fraction:
                        0.005
                            local-volume-fraction-distribution: log-normal
                    missfit-strain: large
                dislocation
                    type: mixed
                    element-density: low
        grain-boundary
            phase: alpha-Al-Li
            angle: high
            impurity: Na K H
            structure-element:
                dislocation
                    type: mixed
                    element-density: high }}
```

Figure 18:   Microstructure of Al-3Li-0.5Mn in Quenched Condition

```
{{ Al-3Li-0.5Mn-pa-strc
    MICROSTRUCTURE-FOR: Al-3Li-0.5Mn-pa
    STRUCTURE-ELEMENTS:
        grain
            size:
                length: 415
            aspect-ratio: 4
                alignment: rolling-direction
            texture:
                copper
                    volume-fraction: 0.02
                brass
                    volume-fraction: 0.02
                S
                    volume-fraction: 0.02
                cube
                    volume-fraction: 0.70
                Goss
                    volume-fraction: 0.24
            recrystallization-level: 100
            phase: alpha-Al-Li
            structure-elements:
                precipitate
                    phase: Al3-Li
                    size:
                        0.03
                            probability-distribution: log-normal
                    aspect-ratio: 1
                    distribution: uniform
                    volume-fraction:
                        0.23
                            local-volume-fraction-distribution: log-normal
                    missfit-strain: 0
                dispersoid
                    phase: Al6-Mn
                    size: 0.2
                    aspect-ratio: 3
                        geometry:
                            rod
                                length: 0.3
                    volume-fraction: 0.005
                    missfit-strain: high
                dislocation
                    type: mixed
                    element-density: low
```

Figure 19: Microstructure of Al-3Li-0.5Mn in Peak Aged Condition

```
grain-boundary
    phase: alpha-Al-Li
    angle: high
    impurity: Na K
    pfz-zone: 0.25
    structure-element:
        dislocation
            type: mixed
            element-density: high
        precipitate
            phase: AlLi
            aspect-ratio: 1
            geometry:
                spheroid
                    diameter: 1
            volume-fraction: 0.04
        missfit-strain: high } }
```

Figure 19, continued

4 Conclusions

This presentation accomplishes the task of representing microstructure information, that is usually communicated in visual form or by natural language, in such a way that the knowledge becomes amenable to artificial intelligence and expert system techniques. As opposed to traditional quantitative descriptions of microstructures this representation does not presuppose the availability of large amounts of quantitative data. Rather, qualitative information that may be obtained through a visual inspection of micrographs or otherwise can be combined with whatever quantitative information is available. Such knowledge corresponds closely to the knowledge used by metallurgists performing alloy design in a commercial R&D setting. We believe that this database architecture can readily be extended to other alloy families and describe a wide variety of microstructures. The general principles may also apply to the microstructure of some non-metallic materials.

5 Acknowledgments

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