

# Knowledge Based Alloy Design

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## Introduction

Alloy design is a metallurgical problem in which a selection of basic elements are *combined* and *fabricated* resulting in an alloy that displays a set of desired characteristics (e.g., fracture toughness, stress corrosion cracking). It is a combinatorially explosive problem dependent upon the choice and amounts of elemental constituents of the composition, and upon the selection, parameterization and sequencing of processing steps.

The quest for a new alloy is usually driven by new product requirements. Once the metallurgical expert receives a set of requirements for a new aluminum alloy, he/she begins a search in the literature for an existing alloy that satisfies them. If such an alloy is not known, the expert may draw upon experiential, heuristic, and theory-based knowledge in order to suggest a set of new alloys that might exhibit the desired characteristics.

The goal of ALADIN is to provide a decision support environment in which expert alloy designers can efficiently explore alternative compositions and thermo-mechanical process sequences. It is important to understand that the search for a suitable alloy design may require many hypothesize/experiment cycles, spanning several years. To reduce the number of iterations, even by one, or to shorten the average time of a cycle would provide significant gains. There are many ways an alloy designer can be supported. First, many alloys have been designed over the last 100 years, with varying properties, which few experts are aware of. By providing a database of alloys it can be determined if a new design is needed. Secondly, by identifying alloys with properties "close to the goal", a starting point for extrapolative design can be found. Thirdly, computational theories exist that link structure, composition and property. Providing easy access to these would aid the alloy designer. Lastly, not all alloy design experts are created equal. Some are more "expert" than others, and their expertise covers different areas of knowledge. Capturing alloy design knowledge used by a variety of specialists in an accessible form would facilitate everyone's design efforts.

A number of issues arise in the construction of a system to aid in the design of alloys. Theoretically, one should be able to determine the properties of an alloy from its microstructure. Practically, the theories are incomplete, requiring the addition of experiential knowledge to fill gaps. As a result, *there exist multiple partial models of alloy design* that relate:

- composition to alloy properties,
- thermal-mechanical processing to alloy properties,
- micro-structure to alloy properties,
- composition to micro-structure, and
- thermal-mechanical processing to micro-structure.

The simplest models of alloys deal only with the relationship between chemical composition and alloy properties. From the point of view of modern metallurgy, only a few structure insensitive properties (such as density and modulus) can be determined with precision from these models. However, empirical (and less precise) knowledge does exist about other properties. Quantitative comparisons, e.g. linear regression, can be made between alloys of varying composition, everything else being equal, which yield some useful quantitative knowledge about properties through regression analysis.

There are also, somewhat more complex, models that describe the relationship between thermo-mechanical processes and properties. Since only composition and process descriptions are needed to manufacture an alloy, it could be assumed that no other models are needed to design alloys. Historically, many alloys have been designed with composition and process models only. Research progress in metallurgy is currently giving new insights into the relationship between the microstructure of alloys and their physical properties. The deepest understanding of alloy design, therefore, involves models of microstructure effects on properties along with models of composition and processing effects on microstructure.

The issues of interest in the ALADIN project thus are: what is the appropriate architecture for the explicit representation and utilization of multiple, parallel models, and how is search in this space of multiple interacting models to be focused?

One particularly important problem is the degree to which design decisions are dependent. Each change in composition or process alters a number of properties. Thus, there is a level of interaction among goals that exceeds the usual situations described in the Artificial Intelligence (AI) planning literature.

Another issue is concerned with representation. Knowledge of the relationship between alloy structure and its resultant properties is at best semi-formal. Much of it is composed of images of microstructure and natural language descriptions. Quantitative models rarely exist, and even when they do, they are often not used.

## The Knowledge Base

Artificial intelligence (AI) has been applied to a number of fields of engineering design. Although there are some features that the various design areas share, such as the need to integrate heuristics with algorithmic numerical procedures, there are also some important differences. Each field of engineering seems to recognize the importance of representing declarative concepts, although specific needs vary. For example, in electrical en-

engineering the representation of components with their spatial and functional relationships seems to be vital. In mechanical engineering, the representation of solid geometric shapes has been studied and is viewed as crucial to the successful evolution of CAD/CAM systems [4, 15]. Materials science identifies the microstructure as crucial to understanding the relationship between the characteristics of materials and composition or processing. A powerful representation of microstructural features is therefore vital to the construction of a materials design support system.

Our representation of declarative metallurgical knowledge demonstrates that qualitative and quantitative knowledge available to the expert in a variety of forms, e.g., tables, diagrams, natural language and pictures, can be given a structured representation that allows the knowledge to be utilized through well known AI techniques. Although many of the AI concepts and approaches used in the representation are routine, the application to the domain of microstructure appears to be novel. In fact, a review of the literature indicates few attempts to define a taxonomy for describing microstructure [9] and no attempts to use a taxonomy of schemata for a computerized knowledge base of microstructure information.

A version of this knowledge base was also used in the development of a corrosion diagnosis system [1]. ALCHEMIST [14] also uses a schematic network to represent plans for designing alloys and methods that define properties and microstructure causality. While our discussion center primarily around aluminum, we are convinced that the framework of the knowledge representation is useful for other alloy families and to some extent even for other materials.

It has been proposed [21] that knowledge representation approaches be judged based on two features: *expressive adequacy*, which includes the ability of the representation to make all important distinctions and to remain noncommittal about details when faced with partial knowledge, and *notational efficacy* that concerns the structure of the representation and its influence on computational efficiency of inferences, conciseness of representation and ease of modification.

In addition, the ALADIN representation was required to meet the following standards:

- The representation should seem natural to materials scientist, to support knowledge base development and maintenance by domain experts.
- The representation should be general enough to support expansion of the system to non-aluminum materials.

These goals and the goals of expressive adequacy and notational efficacy with respect to the domain of alloy design, were considered during the development of ALADIN.

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 [3] are utilized to define relationships and inheritance semantics between metallurgical concepts [6]. The most commonly used relations are ISA and INSTANCE. The ISA relation and some other relations define hierarchies of classes or groups where each higher level sub-

sumes the lower level classes. The INSTANCE relation declares that a particular object belongs to a class or a group and the description of the class serves as a prototype of the instances.

The knowledge base 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.

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 complex representation. The complexity is largely handled by using the meta information features of Knowledge Craft. This enhances the expressive adequacy of the representation by allowing optional finer distinctions. A discussion of phase diagram representations can be found in "Coupling Symbolic and Numerical Computing in Expert Systems" [12].

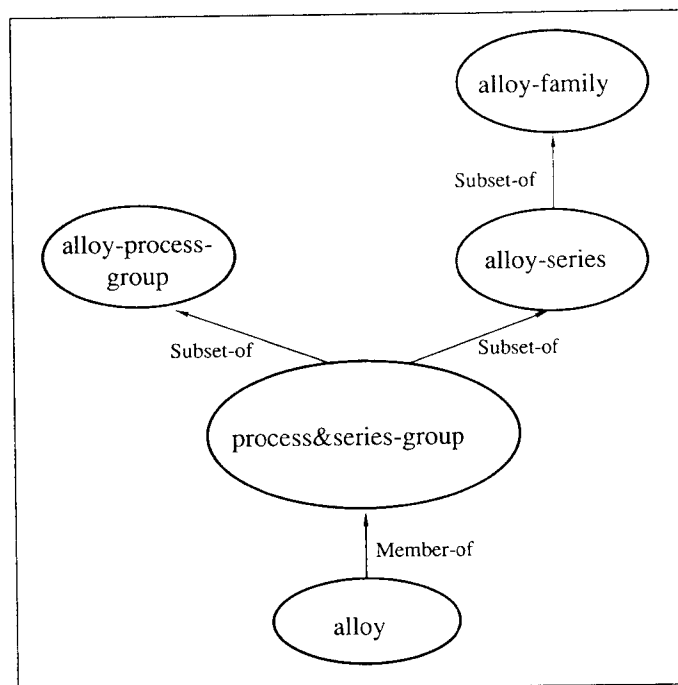


Figure 1: Alloy groups.

### Alloy Hierarchy—Composition, Properties and Processing

Alloys, when viewed from the standpoint of their design, are interrelated and grouped together in a number of different ways. We have defined a number of formal relationships, with different inheritance semantics [6], to enable our schemata to reflect this domain organization. For example, alloys are grouped together into series and families based on composition. They are also related by the processes that go into fabrication (e.g., heat treatment, cold rolling, and tempering), by the

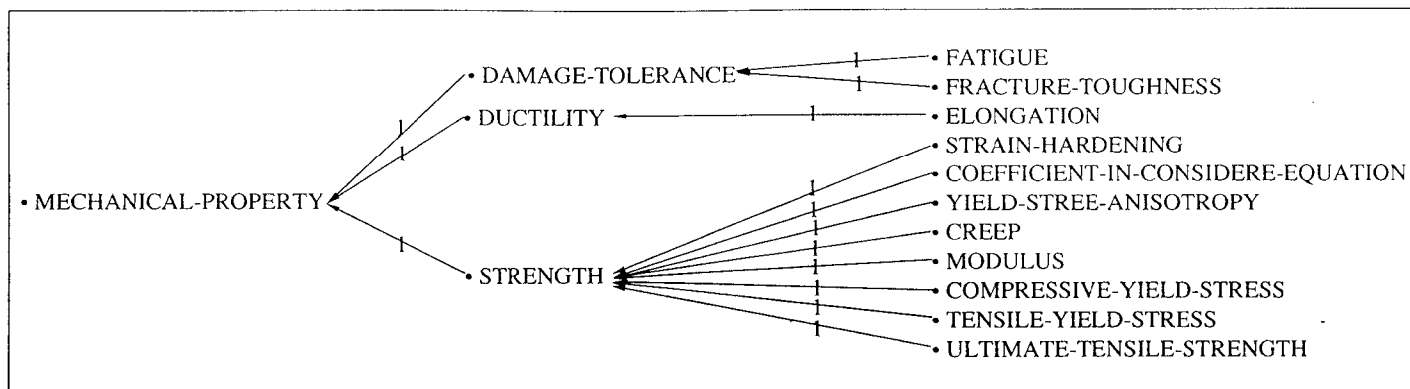


Figure 2: Mechanical property hierarchy.

type of application 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 utilized at various points in the design search in order to make hypotheses and estimates. This is done along a number of different dimensions that define classes of similar alloys, and by looking for trends within these classes.

Figure 1 depicts some of this knowledge-base structure. An **alloy-family** is used to distinguish alloys by primary element, such as aluminum or copper. An **alloy-series** divides a family into subgroups according to secondary elements. An example of a series are those alloys containing AlMgCu. An **alloy-process-group** groups alloys according to processing methods, such as forging or casting. Alloys within a series are further subdivided by their processing to form **process&series-group**.

```

|| 2024-T8-sheet
INSTANCE: alloy
MEMBER-OF: 2xxx-T8-sheet
ADDITIVES: Cu Mg Mn
ELONGATION: 6
...
APPLICATION: aerospace ||
  
```

Schema 1: Typical alloy schema.

A typical alloy schema (Schema 1) will show some of the richness of representations utilized in ALADIN. In this example, the 2024-T8-sheet alloy inherits the following characteristics: (cf. Figure 1, for relationships to general alloy structure):

- The base-element is Al, by inheritance from Aluminum-family, which is an instance of alloy-family.
- The major-alloying-elements are Mg and Cu by inheritance from 2xxx-series-2, which is an instance of alloy-series. (Mn is considered a minor alloying element.)
- The temper is T8, by inheritance from T8-temper-group, which is an instance of alloy-process-group.
- The product is sheet by inheritance from sheet-group, which is an instance of alloy-process-group.

- The process-methods are (in order) cast, preheat, hot-roll, cold-roll, solution-heat-treat, quench, stretch and age. 2024-T8-sheet inherits these values from 2xxx-T8-sheet (an instance of process&series-group), and 2xxx-T8-sheet gets these values from the sheet-group and the T8-temper-group. Since sheet-group is listed before T8-temper-group in the subset-of slot, the sheet-group process-methods come first.
- The modulus is 10.6 and the machinability is B. This is by inheritance from 2xxx-T8-sheet. The alloy could inherit the elongation value of 7 from 2xxx-T8-sheet, but this value is overridden by the value of 6 explicitly listed with the alloy.

A representation for more than twenty physical property measurements has been developed. At the top level of classification, the properties are divided into mechanical, chemical, thermal, electrical, and miscellaneous groups. The classes of mechanical properties are shown in Figure 2.

The classification hierarchy of process methods is used in ALADIN to make inferences about the effects of operations, on microstructure and alloy properties, since groups of methods often have similar effects. **Before** and **after** relations are used to represent time sequences of operations. Figure 3 depicts a portion of ALADIN's process hierarchy.

### Symbolic Microstructure Representation

ALADIN's structure knowledge is split into two categories: microstructure and phase diagrams. Since phase diagrams contain microstructure as well as other geometric information, the microstructure representation will be described first.

Microstructure is the configuration in three-dimensional space of all types of non-equilibrium defects in an ideal phase [9].<sup>1</sup> Such defects are created by thermal and mechanical processing

<sup>1</sup>The phase of a solid material designates its lattice and micro structure. A simple material may exist in three phases: solid, liquid and gas. However, metals often exist in several solid phases, distinguished by different lattice and micro structure, and in the case of alloys also by different composition.

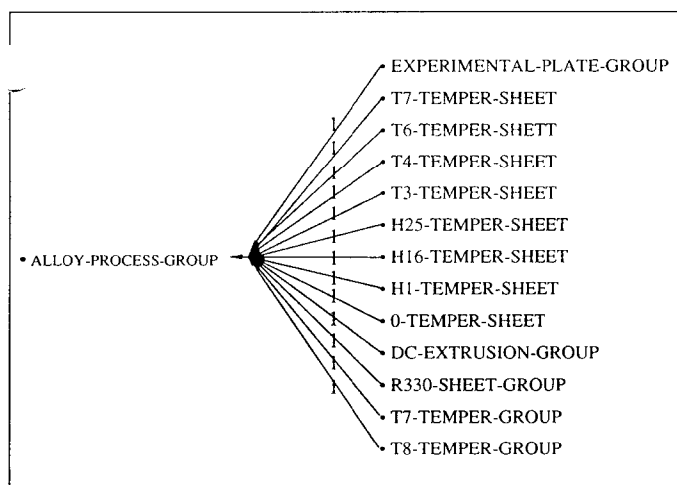


Figure 3: Process hierarchy.

methods, e.g., rapid cooling and cold working. These defects include voids, cracks, particles and irregularities in the atomic planes. These features are called microstructural elements and are visible when the material is magnified several hundred times with a microscope. Metallurgical research has shown that the geometric, mechanical and chemical properties of the microstructural elements, as well as their spatial distributions and interrelationships, have a major influence on the macroscopic properties of the material. The microstructure is often described in abstract, conceptual terms but is rarely characterized numerically. The objective of the microstructure representation in ALADIN is to allow classification and quantification of the microstructure of alloys in order to facilitate the formulation of models that relate the microstructure to the macroscopic properties of alloys.

Much of the empirical knowledge about alloy design involves the microstructure. Which is difficult to represent in a useful way with standard quantitative formalisms. Metallurgists have attempted to describe microstructural features systematically [9] and quantitatively [18], but in practice, neither of these approaches is commonly used. Most expert reasoning about microstructure deals with qualitative facts. Metallurgists rely on visual inspection of micrographs, which are pictures of metal surfaces taken through a microscope. Information is communicated with these pictures and through a verbal explanation of their essential features.

In response to this observation, a symbolic representation of alloy microstructure was created and is a crucial part of the ALADIN database [10]. Figure 4 depicts a portion of the microstructure taxonomy in ALADIN. The two main features of an alloy microstructure are grains and grain boundaries, and these are described by an enumeration of the types of grains and grain boundaries present. Each of these microstructural elements is described in turn by any available information, such as size, distribution, and by relations to other microstructural elements, such as precipitates, dislocations, etc. This representation allows important facts to be expressed even if quantitative

data are unavailable, such as the presence of precipitates on the grain boundaries. Figure 5 shows several types of these elements. Each of these microstructural elements can be further described by its phase, size, shape, volume fraction and distribution, as shown in Schema 3.

### Example of Microstructure Representation

A typical alloy in the ALADIN data base contains a microstructure description that enumerates all microstructural-elements known to exist within the material.

An example of a microstructure [19], is shown on page 24. It is a Micrograph of Al-3Li-0.5Mn in Peak Aged Condition, that is, after solution heat treatment, cold water quenching and peak aging at 400°F for forty eight hours. The corresponding ALADIN representation of the alloy is Schema 2 with the microstructure in Schema 3.

```

[[ 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 ]]
  
```

Schema 2: Representation of Al-3Li-0.5Mn in Peak Aged Condition.

The following information is included in Schema 2:

- The base-element is Al, by inheritance from ExperimentAL-Li-Mn-series, which is an instance of alloy-family.
- The microstructure is described in schema Al-3Li-0.5Mn-pa-strc.
- The alloying elements are Li and Mn as specified in the ADDITIVES slot.
- The process-methods are (in order):
  1. cast
  2. solution-heat-treat at 1020 ° F for 30 hours.
  3. stretch 2 %.
  4. age for 48 hours at 400 ° F, which achieves peak age.

Vasudevan et al. verbally describe the microstructure, referred to as Figure 1(b), as follows:

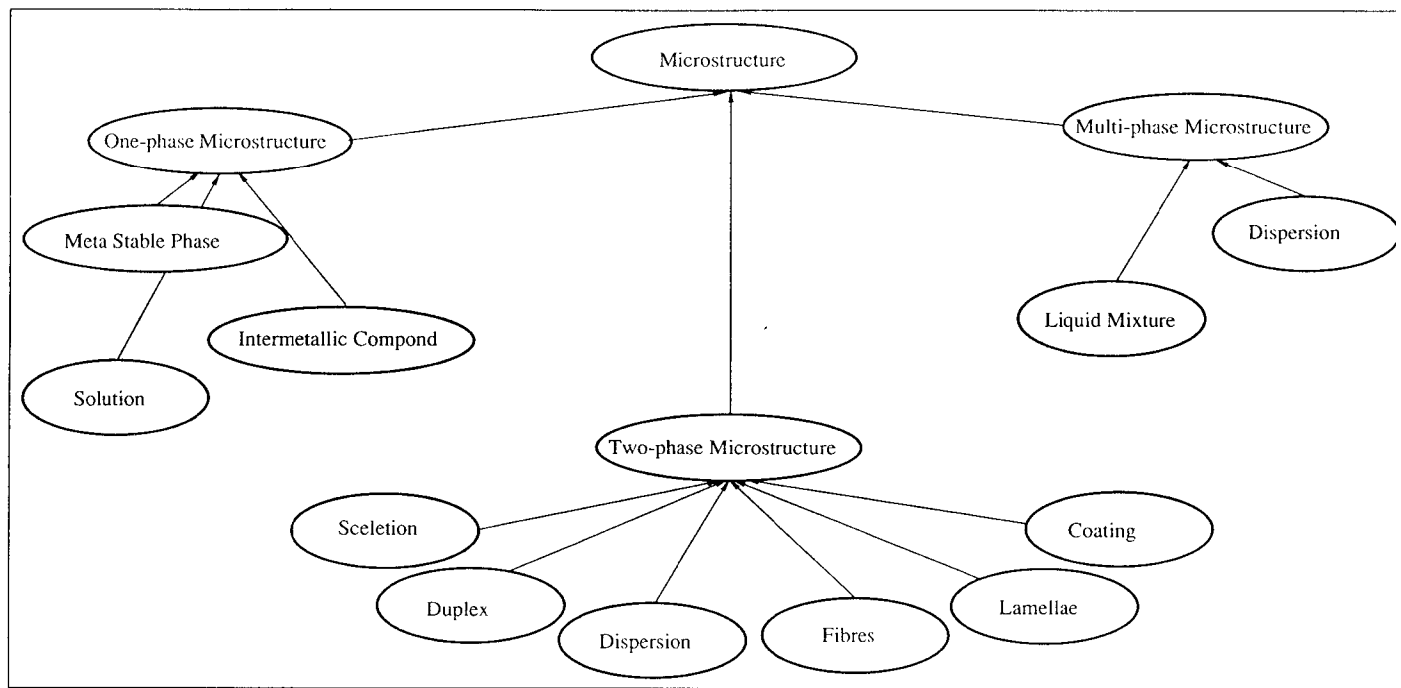


Figure 4: Classification of microstructure.

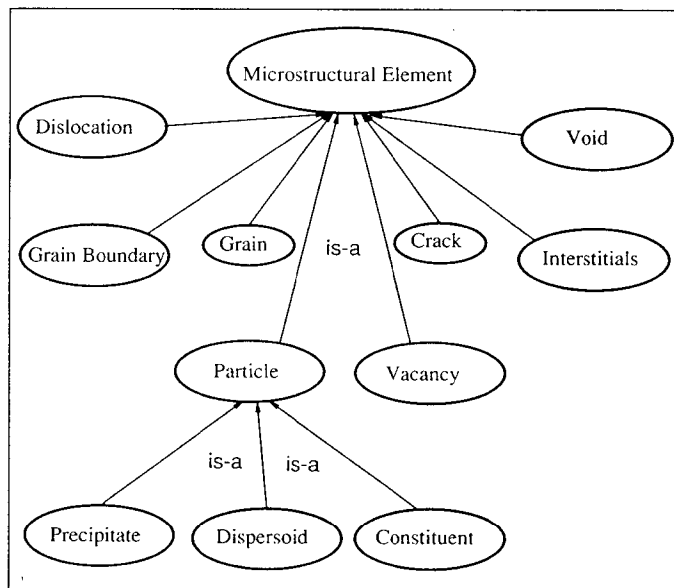


Figure 5: Types of microstructural elements.

"Figure 1(b) shows the microstructure in the peak-aged alloy (condition B), where the strengthening matrix  $\delta'$  precipitates are seen together with coarse grain boundary  $\delta$  precipitates; these are seen as white regions surrounded by dislocations ... and a  $\delta'$  precipitate-free zone (PFZ) 0.5  $\mu\text{m}$  wide which has given up its solute to the grain boundary  $\delta$ ."

The microstructure representation for the alloy, used in ALADIN is shown in schema A1S.

Most of the lithium is in the form of either  $\delta'$  precipitates inside grains or  $\delta$  particles on the grain boundary. Grain boundary has additionally precipitation free zone (PFZ) but other characteristics of the microstructure, such as  $\text{MnAl}_6$  dispersoids, the same as for the SHT case as they are not affected by the ageing treatment. Note that treating grain interior and grain boundary as separate microstructural elements allowed for the association of  $\delta$  particles and PFZ with the grain boundary, a crucial feature in this microstructure. Characteristics of the microstructure such as recrystallization, high angle grain boundaries, elongated grains parallel to the rolling direction and low dislocation density are also represented.

The schema representation is not limited to characteristics that are apparent on a micrograph and includes quantitative information. It is also important to point out that the recursive nature of the representation (i.e., each microstructural element could contain any other microstructural element even one of the same class) makes it possible to represent any imagined microstructure. For example, suppose that the solution heat treated alloy has subgrains inside each grain and that each subgrain consists of several cells separated by dislocations. In ALADIN, such a structure would be represented as grains with high angle boundaries containing small grains with low angle boundaries, which in turn contain even smaller grains (cells) with low or medium dislocation density of the boundaries. Since grains at each "level" can have a variety of microstructural elements, all possible microstructures can be easily represented using this method.

```

[[ 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 distribtn: 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

    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 ]]

```

Schema 3: Microstructure of Al-3Li-0.5Mn in Peak Aged Condition.

Many microstructural elements are associated with a phase, and ALADIN has a phase diagram representation as well. Phase diagrams (Figure 6) represent interconnected systems of phases, where a phase is a state of a metal that holds through a certain range of temperatures and chemical compositions (pressure is not an essential variable in this domain). Different phases in a system naturally fill up a portion of a plane or hyperplane and have boundaries defined by thermodynamic equations and empirical measurement.

ALADIN uses thermodynamic equations, when available, to describe the boundaries of each phase. Often, however, the boundaries are determined experimentally. In this case, each region of an  $n$  dimensional phase diagram may be described as the union of  $(n+1)$ -point lattices in  $n$  dimensional space (see [12] for more details).

## Models

Theoretically, one should be able to determine the properties of an alloy from its microstructure alone. Practically, the theories are incomplete, requiring the addition of empirical knowledge to fill the gaps.

One can view a model as a function which maps from a domain to a range, e.g., from microstructure to properties. Due to incompleteness a model is actually a set of partial functions that are defined across subsets of the domain. Secondly, due to the uncertainty in these models, the domains of the partial functions may overlap and map onto different ranges. Consequently, there is a need to represent not only the partial function, but its domain and the credibility of its result. A set of partial functions and associated information on how to choose a function to apply at each step in the design process can be called a knowledge source. As such, they are similar to the knowledge sources in Hearsay-II [5] where stimulus-response frames define a knowledge source's invoking pattern and possible contribution to the interpretation task.

## Problem Solving Architecture

An alloy design problem begins with the specification of the desired physical properties of the material to be created, expressed as constraints on these properties. The objective of the designer is to identify chemical elements that can be added to pure metal, appropriate amounts as a percentage, and processing methods that can be employed to yield an alloy with the desired characteristics. The line of reasoning that designers mainly use is similar to goal reduction through a hypothesize-and-test cycle. This reasoning starts with abstract choices on microstructure, composition and processing and proceeds towards final determination of percentages for each additive and temperature and duration etc. of all processing steps. Microstructure models provide a powerful guide for the design process since they constrain composition and processing decisions. For example, if meta-stable precipitates should be present, then the percentage of additives must be constrained below the solubility limit, certain heat treatment processes must be applied, and aging times and temperatures must be constrained within certain numerical ranges. Similarly, concepts such as solid solution hardening and interface boundary

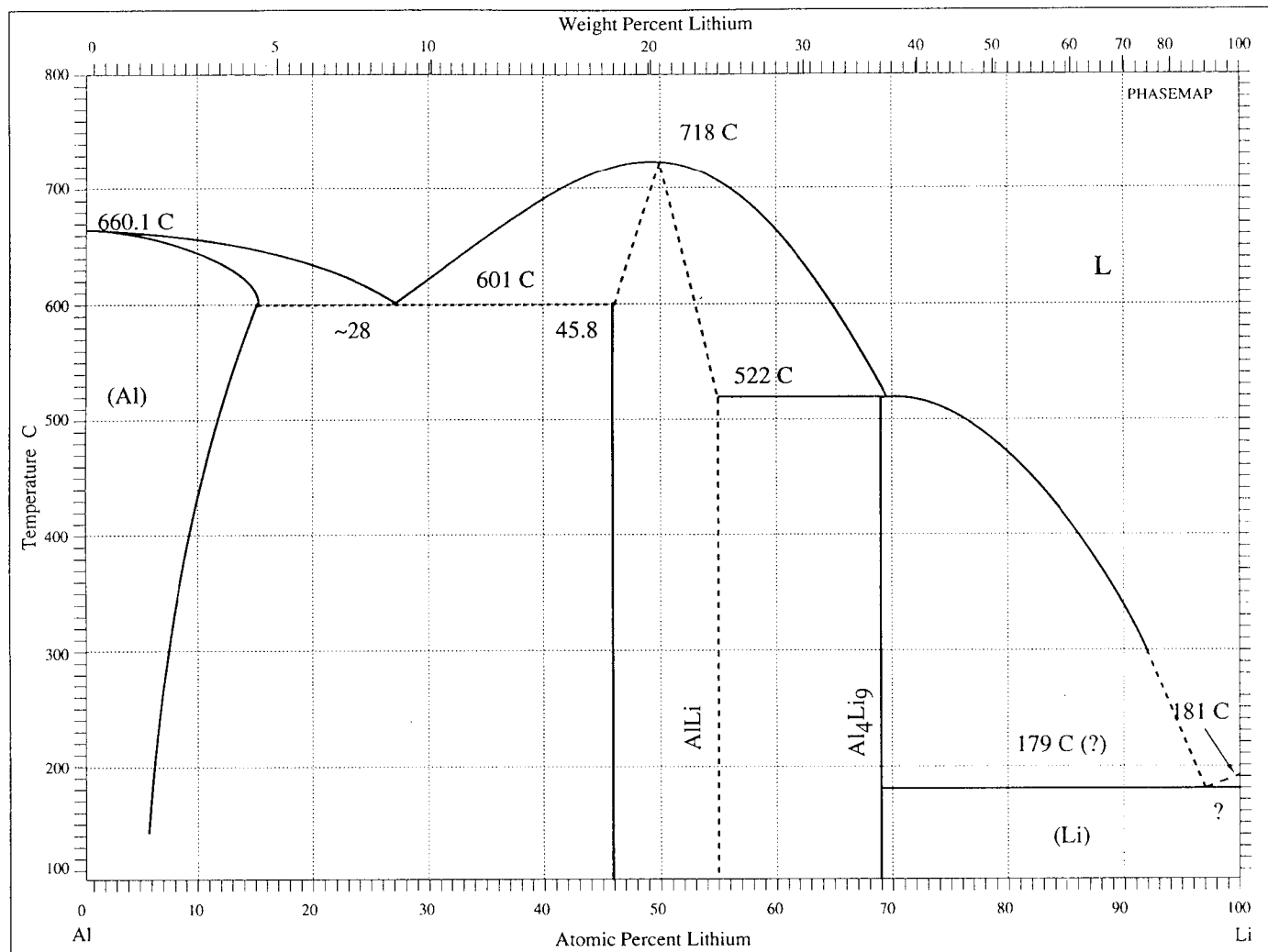


Figure 6: Aluminum-lithium phase diagram.

strengthening are abstractions referring to mechanisms that can involve a range of additives and process methods, but nevertheless narrow subsequent qualitative and quantitative choices. Earlier or later, depending on the nature of the design task and the style of the designer, a known material is selected as a base line or starting point. The designer then alters the properties of the known material by making changes to the composition and processing methods. The effects of these changes on the various physical properties are estimated, and discrepancies are identified to be corrected in a later iteration.

However, a detailed study of metallurgical reasoning reveals a number of complexities which must be taken into account. First, knowledge is often applied in an opportunistic fashion. This is a consequence of the existence of multiple, but incomplete, models, e.g. it is rarely feasible to predict properties quantitatively from microstructure, but given the class of microstruc-

ture, semi-empirical models can often be used to predict properties from composition and processing parameters. Second, the strategies that designers use to select classes of knowledge to be applied vary among individuals. For example, in the selection of the baseline alloy to begin the search, some designers like to work with commercial alloys and others prefer experimental alloys produced in a very controlled environment. Still others like to begin with a commercially pure material and design from basic principles. Third, when searching for alternatives to meet target properties, some designers construct a complete model of the microstructure that will meet the properties and then they identify composition and process options. Other designers prefer to think about one property at a time, identifying a partial structure characterization and implementation plan that will meet one property before moving to the next. Still other designers prefer to avoid microstructural reasoning altogether by using direct relationships between design variables and design targets. Fourth, all designers

asionally check their partial plans by estimating the primary and secondary effects of fabrication decisions on structure and properties. The frequency of this activity and the level of sophistication of the estimation models varies among designers.

### Planning and the Design Process

The ALADIN architecture has been designed to support opportunistic reasoning, at different levels of abstraction, across multiple design spaces. A multi-spatial reasoning architecture akin to a blackboard model [5, 8] was chosen. There are five spaces:

1. **Property Space:** The multi-dimensional space of all alloy properties, (e.g., tensile strength, ductility, fracture toughness).
2. **Structure Space:** The space of all alloy microstructures.
3. **Composition Space:** The space where each dimension represents a different alloying element (e.g., Cu, Mg).
4. **Process Space:** The space of all thermo-mechanical alloy manufacturing processes.
5. **Meta Space:** The planning space that directs all processing. The meta space holds knowledge about the design process and control strategies. Planning takes place in this space in that goals and goal trees are built for subsequent execution.

The spaces are subdivided into levels that correspond to different degrees of detail, from abstract qualitative concepts to numerical quantities. The highest level of the composition space identifies which elements are to be added. Lower levels identify the quantity to add of each element.

Activity is generated on different planes and levels in a way similar to Stefik's MOLGEN system [17]. Planes contain one or more spaces. ALADIN's planes are:

1. **Meta** or strategic plane, which plans for the design process itself, establishing sequencing, priorities, etc.
2. **Structure** planning plane, which formulates targets at the phase and microstructure level, in order to realize the desired macro-properties
3. **Implementation** plane, encompassing chemical composition and thermal and mechanical processing.

Search activity aims at reducing the number of outstanding goals through an hypothesize-and-test paradigm. Partial models propose and verify hypotheses at all levels of abstraction connecting two or more spaces of knowledge. For example, the models linking structure and composition can propose alloying elements in the composition space which yield a structure specified in the structure space. In the opposite direction, a model can predict properties of a proposed composition, by checking whether there would be a phase change in the structure space.

The qualitative and quantitative levels of the Structure, Composition and Processing spaces are activated as appropriate, to generate hypotheses that specify design variables in their own range of expertise. Hypotheses generated on other planes and levels constrain and guide the search for new hypotheses. An existing qualitative hypothesis obviously suggests the generation of a quantitative hypothesis. Certain microstructure elements

can be produced by compositional additives, while others are produced by specific processes with the composition restricting the choices available.

Ideally, the alloy design process starts in the structure space where decisions are made on microstructural features that imply desirable properties. These decisions are thereafter implemented in composition and process space. Since models are incomplete the appropriate sequence of execution is not known *a priori*. Consequently, the system must select, from the opportunities available, the most appropriate model at each decision point.

The degree of opportunism exhibited by the system is determined by the meta-level planner. Its basic cycle is:

1. Select a hypothesis to extend, based upon its credibility
2. Evaluate it relative to the target properties
3. Select a property to improve
4. Select a model which will optimize the chosen property by refining the hypothesis into new hypotheses
5. Evaluate how well the new hypotheses meets the selected property goal

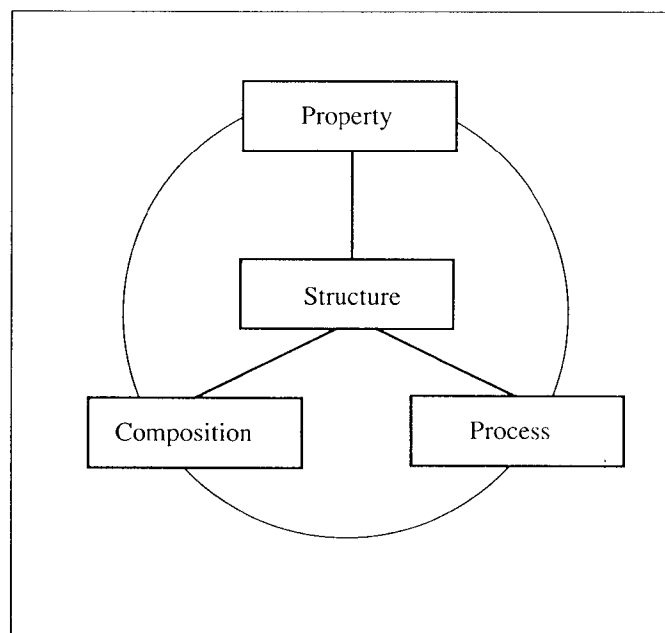


Figure 7: Spaces of domain knowledge.

In practice, sequencing among these steps is more flexible when demanded. For example, the selection from among a set of new hypotheses often requires that they be evaluated in detail. Decisions about sequencing at this level are made in the meta space. Within the steps in the hypothesize-and-test cycle, there is a sequence of reasoning based on the causal relations represented by links in Figure 7. For instance, in order to evaluate the current hypothesis, the effects of composition and process decisions on microstructure are determined. These microstructure estimates are then used to determine the physical

cal properties of the alloy. When generating a new hypothesis, on the other hand, causal relations are examined in the reverse direction. Given the target physical properties, microstructure and then composition and process alternatives are identified. In the case when microstructure knowledge is not available, the system may search for weaker models, such as process-property relations, that bypass the microstructure plane, utilizing the existence of several models.

The selection of goals to satisfy, and the hypotheses and models to satisfy them is performed by the planner in its basic hypothesize and test cycle. Several types of information are used in making such decisions, including:

- the status of the search,
- the history of the solution process,
- constraints on strategic alternatives, and
- the effectiveness of various strategic alternatives.

The status of the search is characterized by the constraints, hypotheses and estimates that have been created. These indicate what problems remain. The history of the solution process is retained in the goals. Given these sources of information, constraints on control alternatives are easily represented in rule form. Some examples are:

```

If numerical decisions regarding
  composition and process
  have not yet been made,
Then quantitative evaluation models
  can not be applied;

If decisions have not yet been made
  regarding what processing
  steps to use,
Then it makes no sense to reason about
  temperatures and rates.

```

The system also has a notion of what strategies will have the greatest impact on the search, based on heuristic knowledge obtained from metallurgists. Rules include:

```

If it is possible to reason about
  microstructure, composition
  or process,
Then microstructure reasoning is
  preferred;

If many fabrication alternatives have
  been identified to meet a single
  target,
Then use simple heuristics to evaluate
  each and prune the search.

```

Due to the complex interdependence of design decisions on an alloy's final properties, simple concepts of goal protection are inadequate [20], and a least commitment strategy that minimizes goal interaction is employed.

ALADIN begins in the meta space and frequently returns there for new direction. When the meta space is activated, strategy rules identify activities that are reasonable and create top level

goals with appropriate context, space, and level information for those chosen activities. Often, several alternative strategies are possible at any point in the search, and the user is offered a menu of possibilities. The system recommends the strategy that is estimated to be most effective. After the user accepts or overrides this selection, the meta rules expand the goals by creating more detailed subgoals. These goal trees constitute a plan for accomplishing the requested activity. Control then returns to the domain spaces, which process the goals until their success or failure is determined. At that point, control returns again to the meta space. Alternation between meta and domain spaces continues until the problem-solving process is complete.

Within the meta space, numerous design strategies (obtained from different people) are integrated into a single system. As a result, ALADIN can develop several solutions to a single problem by applying different approaches. Flexible user control allows a metallurgist to experiment with different strategies. The user may, in fact, explore solutions arising out of the application of hybrid strategies that are not usually applied to a single problem.

### Reducing Search Complexity

The partial models available to ALADIN have the potential to generate an exponentially large set of alternative designs. In order to reduce the search complexity, ALADIN employs the techniques of:

- hierarchical search,
- least commitment search, and
- constraint directed search.

**Hierarchical search.** Many of the spaces are divided into levels higher levels being abstractions of lower levels. For example, in the composition space, the highest level is used to specify whether an element is to be added or not. Lower levels specify the amounts of the element to add. In the structure space, the highest level specifies the type of phase while the next lower level specifies the types of microstructural elements present in the microstructure. Still lower levels may contain quantitative information on the microstructure. Planning begins by making decisions at the abstract level, and then gradually made more precise, allowing global consequences of decisions to be evaluated before effort is spent in detailed calculations.

Metallurgical models act as a partial filter on design decisions. That is, when decisions about composition and process are made, they are filtered through the structure space in order to predict their effects in the property space. The filter is partial since there may not exist an appropriate metallurgical model in all cases. Consequently, microstructure decisions serve as an abstract plan that cuts down the number of alternatives in the composition and process spaces. In this way the role of the microstructure differ in some respects from abstract planning as described by Sacerdoti [16]. The main differences are:

- Microstructure concepts are distinct from composition and process concepts, not merely a less detailed description.
- The microstructure plan is not a part of the final design, since an alloy can be manufactured with composition and process information only.

- The microstructure domain is predefined by metallurgical expertise, not defined during implementation or execution of the ALADIN system.

These differences lead to the following contrasts with a MOLGEN-like system:

- Instead of one hierarchy of plans there are three (structure, composition and process), each of which has abstraction levels.
- Since structure decisions do not always necessarily have the highest "criticality" (as defined by [16]), opportunistic search is important.
- The effect of abstract hypotheses is more complex because decisions in the structure space cut the search by constraining the choice of both composition and process hypotheses. The existence of more than one level in each space also introduces new types of interactions.

**Least commitment.** Given the fact that most design decisions affects more than one target property, it would be inappropriate to make precise commitments early in the design process. Quantitative hypotheses are therefore expressed as constraining inequalities which are kept as broad as possible. A hypothesis is refined by posting additional constraints that reduce the region for the design variables. This strategy reduce the need for backtracking in selecting values. ALADIN's domain lends itself very readily to this technique: Qualitative reasoning can be used to determine what types of constraints need to be considered and most numerical variables admit to ranges of values.

**Constraints.** Though ALADIN focuses on a single property in the hypothesize-and-test cycle, it uses constraints to tie properties together so that it does not spend time exploring a decision path which would negate other properties. (Constraints are represented as Lisp expressions involving any function or variable, which must evaluate to a non negative result.) The formulas for density and modulus immediately yield constraining equations, and constraining equations for other properties can be obtained by regression in the alloy database. Some variables, like temper, are not easily quantifiable, but have an indirect impact on the generated constraints. Temper information, for example, is used to select the alloys in the regression. Another source of constraining equations are the phase diagrams, several heuristic rules involving phase boundaries and solubility limits. In the evaluation phase, all constraints are tested to see if the design is acceptable not only with the current goal but, with the other property goals.

In some cases, constraints are used not only to evaluate decisions, but to generate decisions. A variant of the gradient method described by Hadley [7] is used to find a feasible point for a system of nonlinear inequalities.

## Model Based Inference

Experience from interaction with metallurgists and insights gained during the work with the ALADIN system suggested that there is a need for an alternative mode of operation. The typical user of an alloy design system will, for the foreseeable future, be a metallurgist with considerable expertise in at least

some aspects of alloy design. Each metallurgist has a certain style (and often firm opinions) on what approach should be taken. A metallurgist may, therefore, sometimes be better served by a system that leaves the top control to the user, but assists the design by making a menu of operations available. That is the purpose of the Design Assistant mode. In this mode the metallurgist guides the search in the direction he wants. The elaboration of hypotheses is also put under user control by making available to the user a set of models which can be used to derive new information.

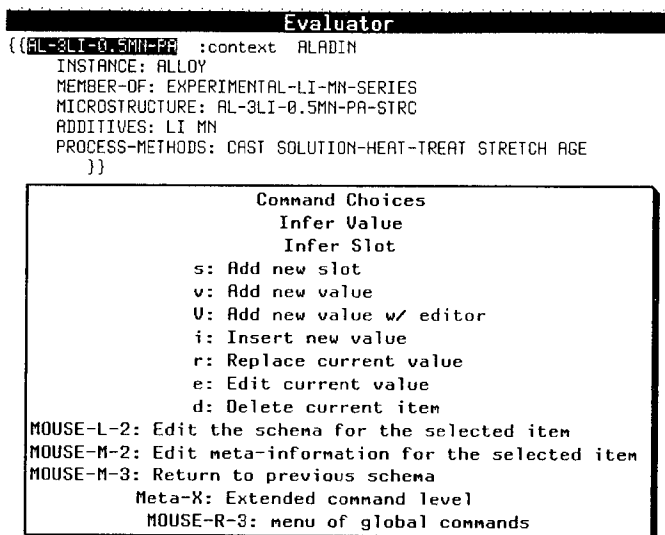


Figure 8: The Infer Value and Infer Slot items can be selected.

The Design Assistant applies the very general and powerful notion of models. A schema based representation of models and a domain independent inference engine that invokes models to infer values of attributes in schemata was created [11]. Domain dependent information, facts, qualitative and quantitative models, as well as much of the domain independent control knowledge, is uniformly represented in schema form.

The reasoning process involves inferring attribute values in existing or newly created schemata. If acceptable values can be obtained through simple retrieval, with or without inheritance, the value is considered known and no model needs to be invoked. Otherwise a value will be inferred, if possible, through a search for the "best" model that yields an acceptable result. The selection of models is done in three stages. First the domain of validity of the model is determined. The domain of validity is a subset of all schemata specified with the CRL restriction grammar [3], e.g., the DOMAIN attribute in Schema 4 limits the use of that model to the temperature of (meta-)schemata that are of CLASS artificial. Second, the valid models are ranked by determining their credibility. Third, the value generated by the model has to satisfy range and cardinality restrictions, e.g. the DOMAIN of Schema 5 must be one or two of (type class natural) and (type class artificial).

The search and ranking of models, as well as the determination

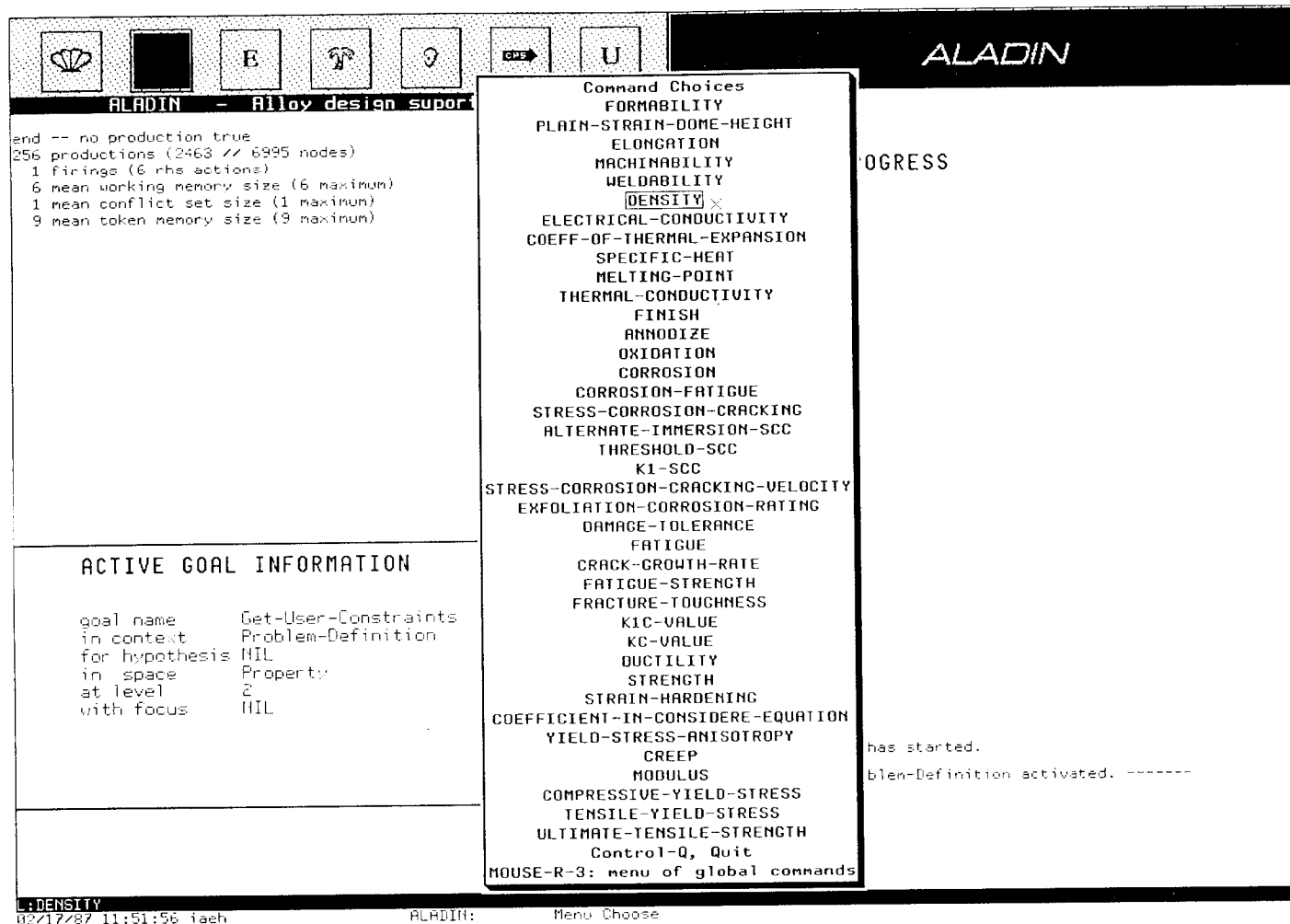


Figure 9: The user is presented with a menu of properties to constrain and will be given the opportunity to limit each selected property quantitatively.

of domain, credibility and range, are inferences that can be performed by control models. The system has a set of domain independent control models that can be augmented and superseded by domain dependent control models whenever appropriate.

The simplest use of a model to infer the value of a specific slot in a schema is to take the value from the same slot of another schema that is in some sense similar. This schema then becomes a model or an analog of the first schema. To take a simple example, if one wants to determine the aging temperature for the alloy represented by Schema 2, then one could use knowledge about the typical temperature for artificial aging (see Schema 4) as a model and assume that the temperature is 400 degrees Fahrenheit. The Schema AGE-TEMPERATURE-DEFAULT-MODEL is declared to be a model of temperature through the relation MODEL-OF.

```

Evaluator
((AL-3LI-0.5MN-PA :context ALADIN
  INSTANCE: ALLOY
  MEMBER-OF: EXPERIMENTAL-LI-MN-SERIES
  MICROSTRUCTURE: AL-3LI-0.5MN-PA-STRC
  ADDITIVES: LI MN
  PROCESS-METHODS: CAST SOLUTION-HEAT-TREAT STRETCH AGE
  DENSITY: 0.098
))

```

Figure 10: The Infer Value item gives the result.

Algorithmic and numeric models can be introduced through procedural attachment, i.e., by attaching a piece of code to attribute, that generates a value. The Schema 5 is a model that invokes a procedure specified by the AGE-TEMPERATURE-MOI PROCEDURE schema.

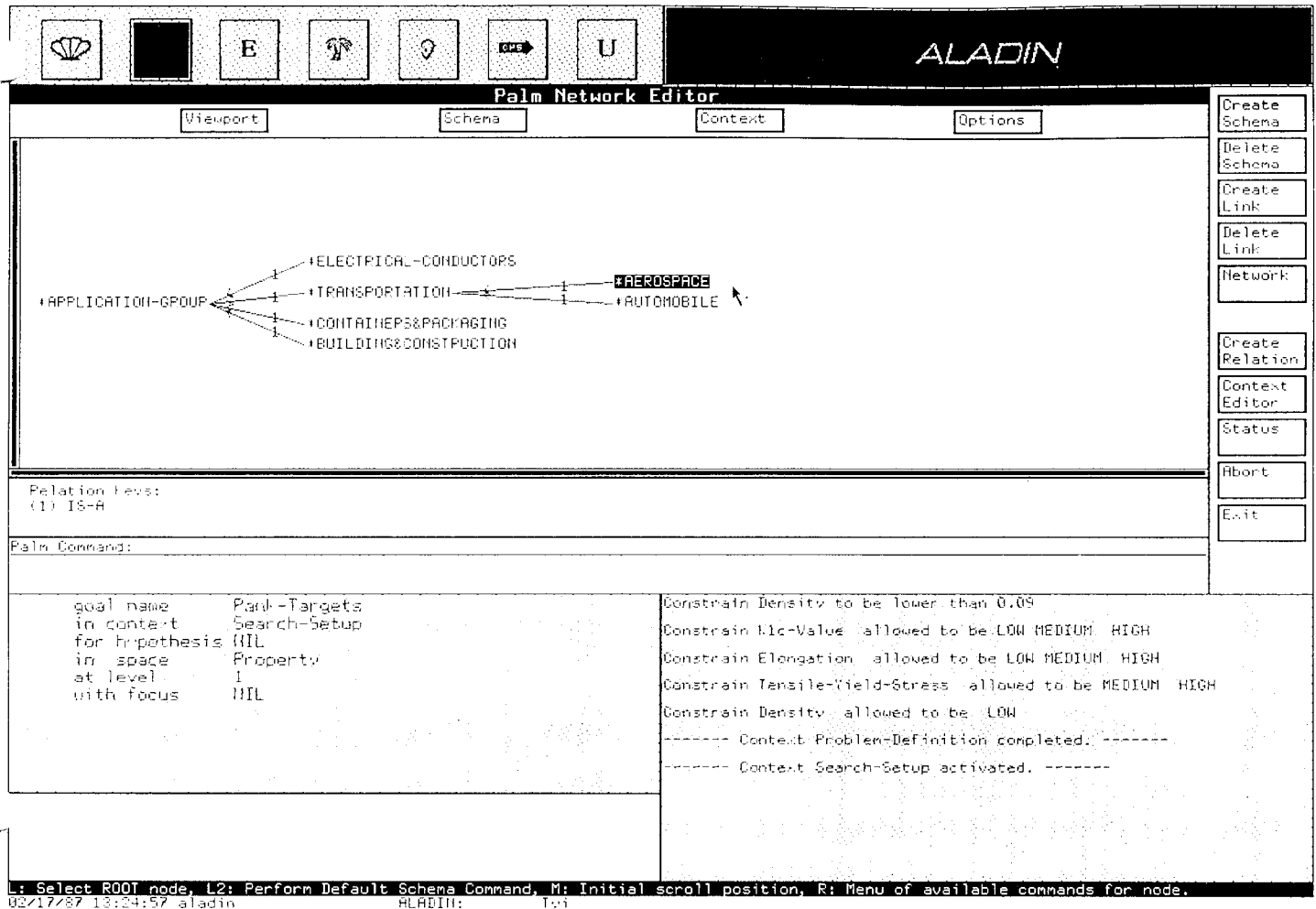


Figure 11: Property priorities are largely determined by the application, e.g., selecting aerospace applications will give density the highest priority.

The system described here can be thought of as an extension of the features of more conventional schema representations, and is implemented as a function (infer-value) to be used instead of the function provided by the schema representation system (get-value). This system allows representation of more than one possible value, or lists of values, for an attribute. The mechanisms for searching and selecting models of attributes makes it possible to distinguish cases based on complex criteria, e.g., numerical relationships. The range and cardinality checks on inferred values implements a simple backtracking feature. Successfully inferred values are optionally stored in the schema, with meta information on their source. Hence, if the same call to the infer-value function is repeated, the value will be obtained by simple retrieval. This is also true about input data and intermediate results obtained by recursive calls to the infer-value function either by the selected model or the infer-function itself.

If a convention is adopted to store only facts as regular values, and represent default values as models, then this architecture provides a clean cut between defining properties and default properties, which is a well known problem in knowledge representation [2].

The design assistant allows the user to invoke models and enter information in an interactive environment. The environment is similar to the Knowledge Craft schema editor and includes simple editing commands. Figure 8 shows the menu of top level commands. Selecting the Infer Slot command generates a menu of slots, i.e., attributes, that are appropriate in the displayed schema. In this case the menu would look much like the one in Figure 11.

Selecting an attribute introduces it in the displayed schema. The Infer Value command activates the inference engine described above and inserts the resulting value. Figure 10 shows the result of inferring the density.

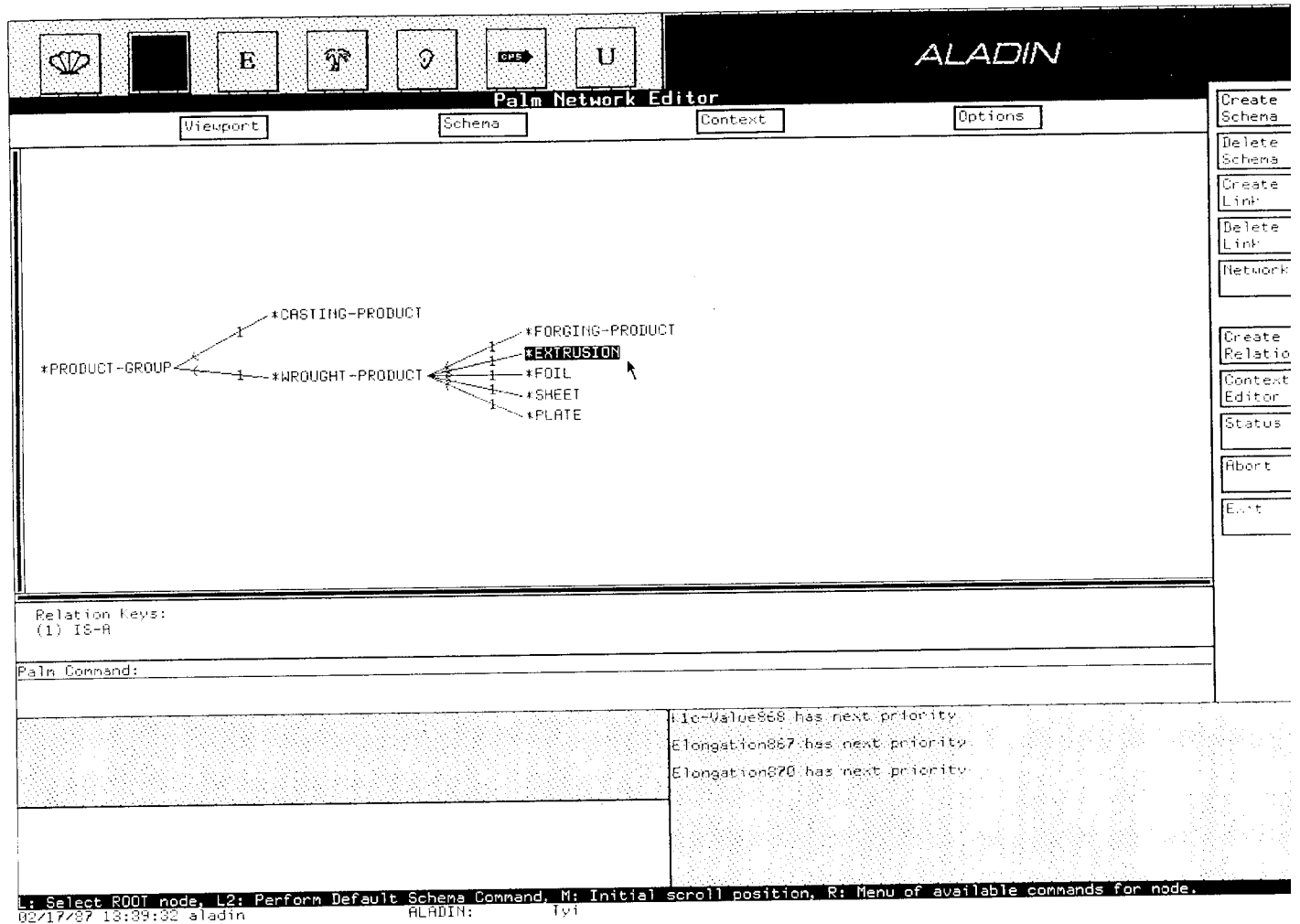


Figure 12: The user may select the product form of interest.

## The Prototype

ALADIN runs on a Symbolics LISP Machine under Genera 7.1 within the Knowledge Craft 3.1 [3] environment at a speed comfortable for interaction with expert alloy designers. The design run outlined in this section takes about half an hour, and involves considerable interaction with the user, whose choices influence the quality of the outcome. The system is at the mature, advanced-prototype stage, where it can begin to assist in the design process, particularly as a knowledge base and as a design evaluator. These are two of the main modes of use that we set out to develop, with independent design and discovery being the third mode. We must point out, though, that the knowledge base is presently focused on narrow areas of alloy design, with expertise on only three additives, two microstructural aspects, five design properties. Some heuristic rules are *ad hoc* rather than integrated into the strategy-planning-implementation hierarchy. We have dealt in depth only with ternary alloys. But these restrictions are by our own choice, so

```
(( AGE-TEMPERATURE-DEFAULT-MODEL
  ISA: model
  MODEL-OF: temperature
  CREDIBILITY: 0.2
  DOMAIN: (type class artificial)
  TEMPERATURE: 400 ))
```

Schema 4: Schema representation of a model of typical aging temperature.

```
(( AGE-TEMPERATURE-MODEL
  ISA: model
  MODEL-OF: temperature
  CREDIBILITY: 0.9
  DOMAIN:
    range: (or (type class natural) (type class artificial))
    cardinality: (1 2)
  TEMPERATURE:
    demon: age-temperature-model-procedure))
```

Schema 5: General age temperature model.

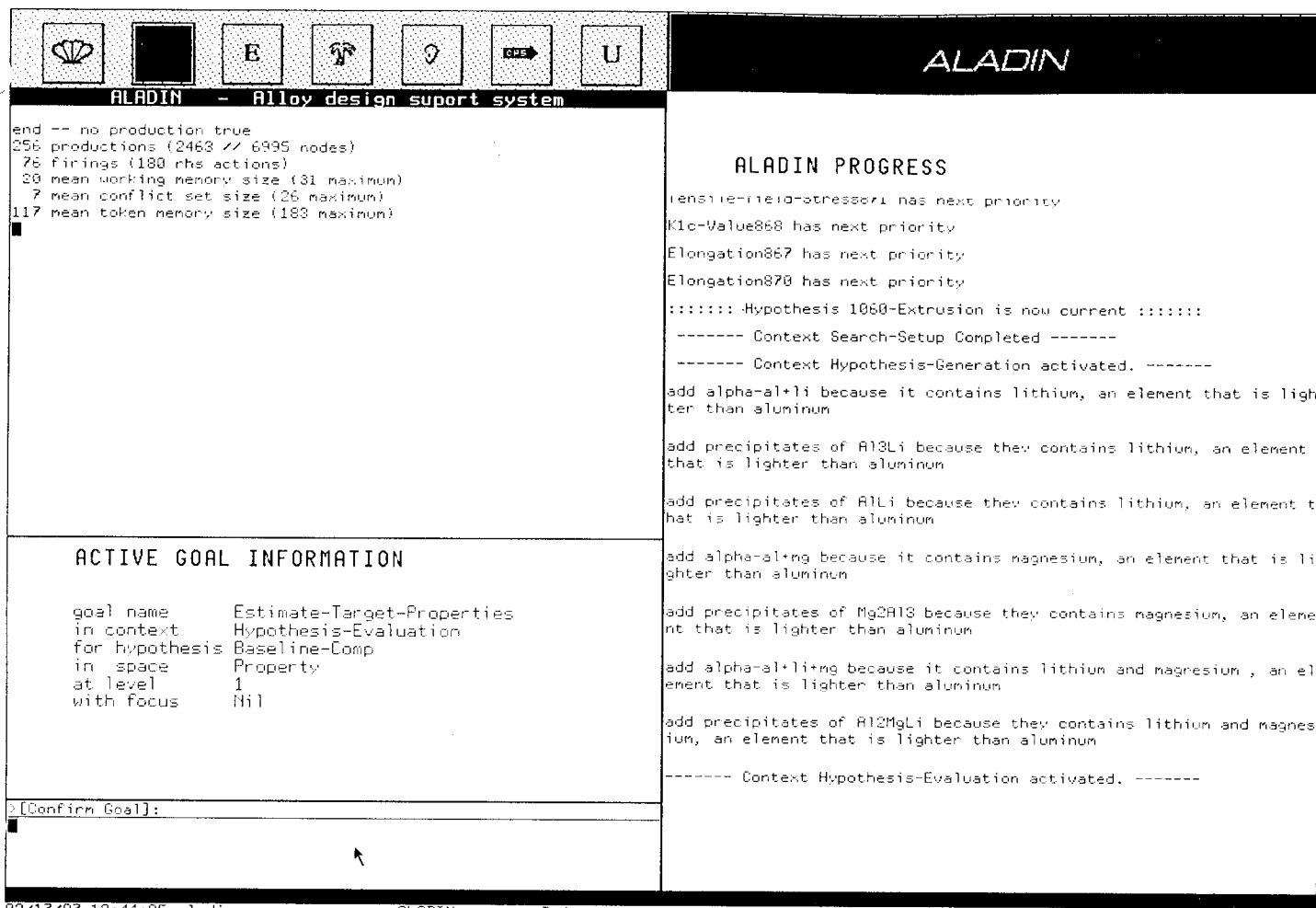


Figure 13: In this example, six hypotheses on the microstructural composition are generated, all involving light elements in response to a low density target.

that we can concentrate on the selective areas of greatest importance to our expert informants and sponsors. Within these restrictions lie a number of commercially important alloys, whose rediscovery by ALADIN would be a major milestone.

The first goal of ALADIN is to obtain a target for the desired alloy. A design target is generally described in terms of target values on various physical properties. The user therefore specifies these property targets early in the design run (Figure 9). These targets act as constraints on the target alloy.

Since the search for a new alloy usually is driven by product requirements, the designer will usually have an application in mind. As shown in Figure 11, the user may select an application and this information is used by the system to select a strategy for the design. ALADIN pursues one target at a time and therefore needs to prioritize them.

The system uses its database of known commercial and ex-

perimental alloys for qualitative and quantitative comparisons to the target. Such comparisons are best made between alloys of similar product forms; Figure 12 shows how product forms can be selected.

Once the problem is defined and the search is set up, a cycle of hypothesis generation, selection and evaluation is entered. Figure 13 shows a generation phase.

In Figure 14 only a qualitative evaluation, is performed. The subsequent selection phase assigns credibilities to the alternative hypotheses to form a basis for selection. In this case no quantitative constraints are available that could have an impact on the selection.

The hypothesize, select and evaluate cycle adds details of the design incrementally and builds a tree of hypotheses as shown in Figures 14-17. The final result of a design session is a partial description of an alloy in the form of schemata using the knowledge representation of the alloy data base.

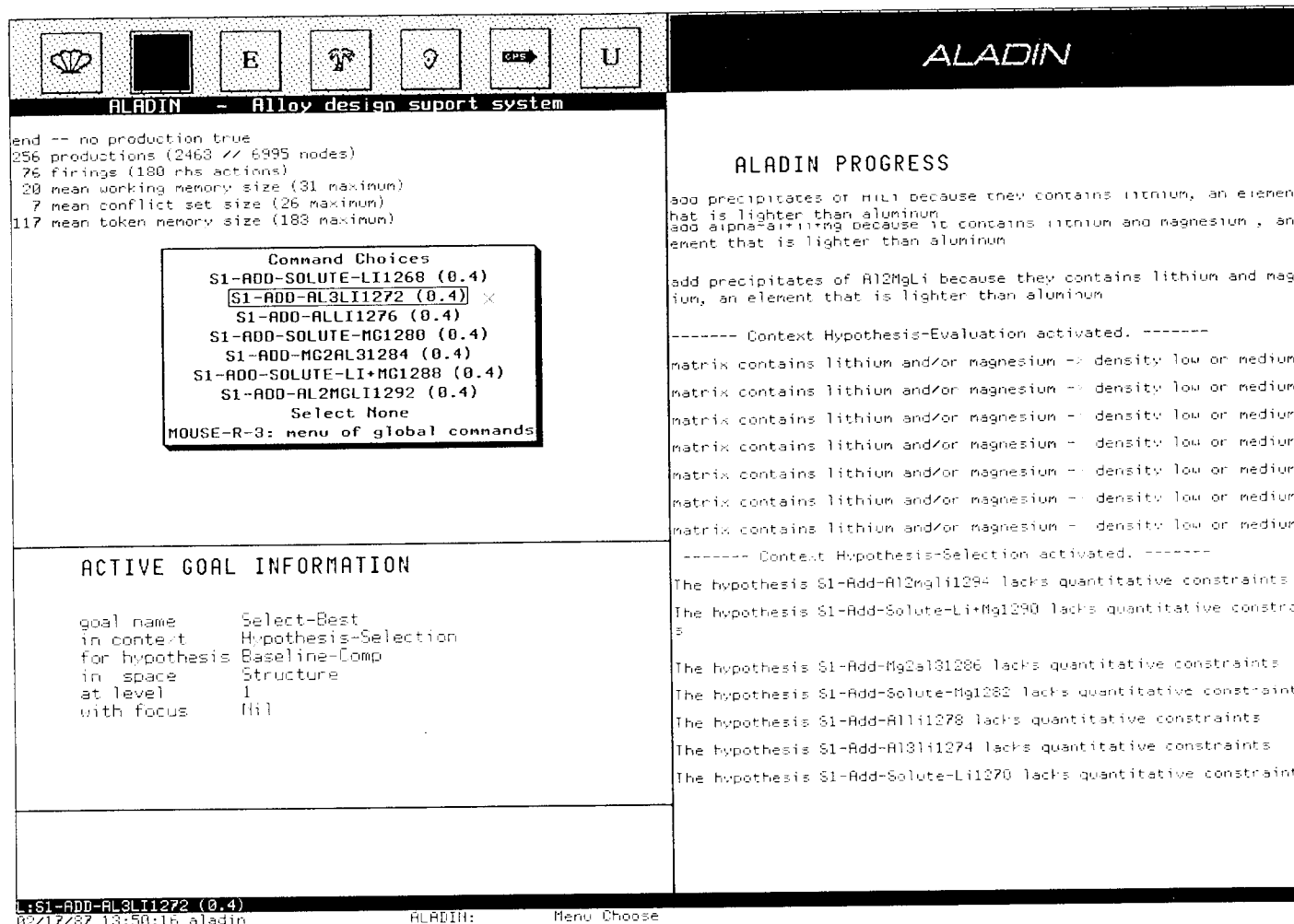


Figure 14: A qualitative evaluation that notices the fact that the addition of light elements implies low density, is performed. A menu of hypotheses allows the user to force a selection.

## Conclusions

Alloy design is thought to require too high a degree of creativity and intuition for automation. However, we have found that hypothesize-and-test, abstract planning and rule-based heuristic reasoning can reproduce a significant portion of the reasoning used by human designers on prototype cases. The metallurgists working with us on the system have concluded that the representation and reasoning are sufficiently powerful to warrant the expansion of the knowledge base so that it can be used on a routine basis. (The current ALADIN system has approximately 2400 schemata, 250 CRL-OPS rules, and 200 lisp functions.)

ALADIN's major accomplishments include:

- providing a representation in which multiple partial models can be represented declaratively;
- formulating an architecture in which incomplete and

even inconsistent models can be integrated in the design process;

- satisfying multiple interacting goals by determining local commitment constraints.
- developing a framework and applying a set of techniques that allow effective coupling of symbolic (qualitative) and numerical (quantitative) reasoning, within a structure containing various representations of information;
- finding ways to reason qualitatively with constraints that are expressed quantitatively;
- providing an interactive environment where the expert can share control of the design process with the system.

The overall goal of ALADIN as an industrial application of techniques has been to make the process of alloy design more productive [13]. This process, as currently practiced, involves several iterations over the course of five years. We are confident that a tool such as ALADIN can achieve significant productivity gains.

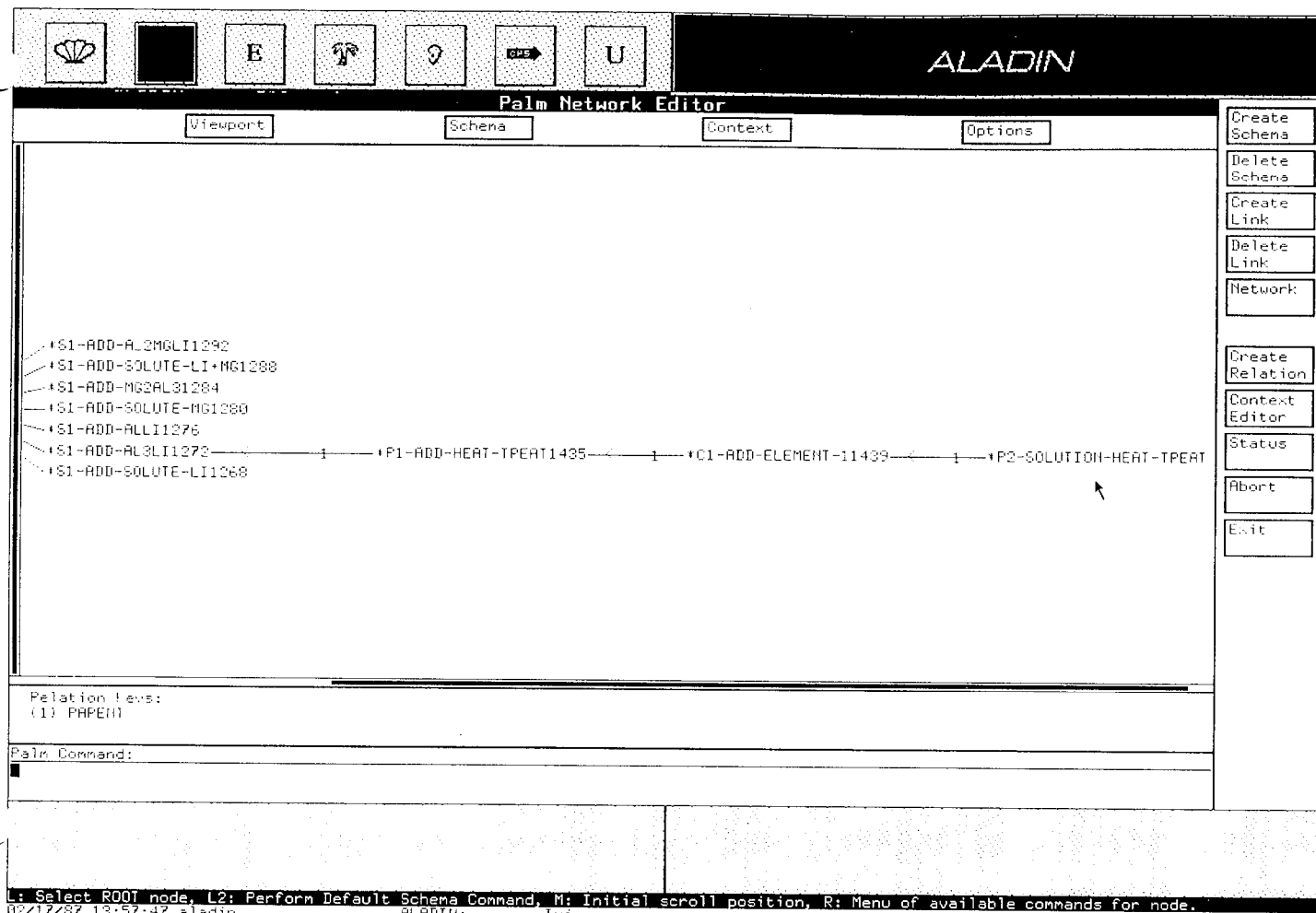


Figure 15: Hypotheses on heat treatment and composition are added.

improvements and aid in the discovery of better alloys. It can do this by making the generation of alloying experiments more systematic, by aiding in the evaluation of proposed experiments, and by allowing individual designers to supplement their own specialized expertise with that of the program, which is a pool of expertise from various sources, helping to fill in gaps where a specialist may be weak.

The complexity of the domain has given us the opportunity to extend the frontiers of artificial intelligence research. We feel that search in the space of abstract models (in our case, microstructure), has potential applications in other design areas as well, such as the design of other metallic or nonmetallic materials, and in general, designs that are dominated by non-geometric constraints and require a combination of qualitative and quantitative reasoning. We also feel that our representation of strategic knowledge, with flexible user control, is a powerful way of combining knowledge from multiple experts into a single system. We hope that these ideas will be useful to developers of future expert systems.

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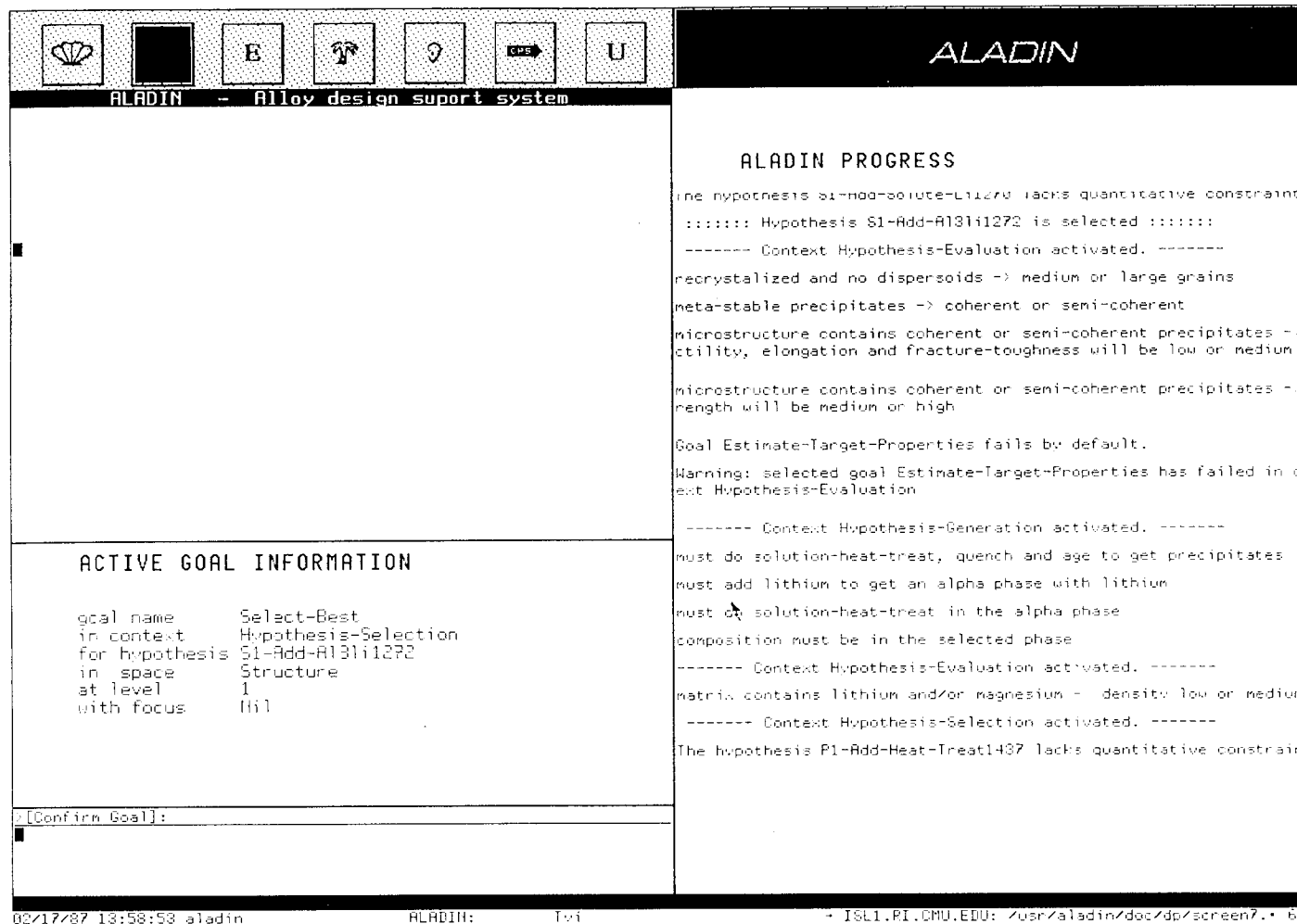
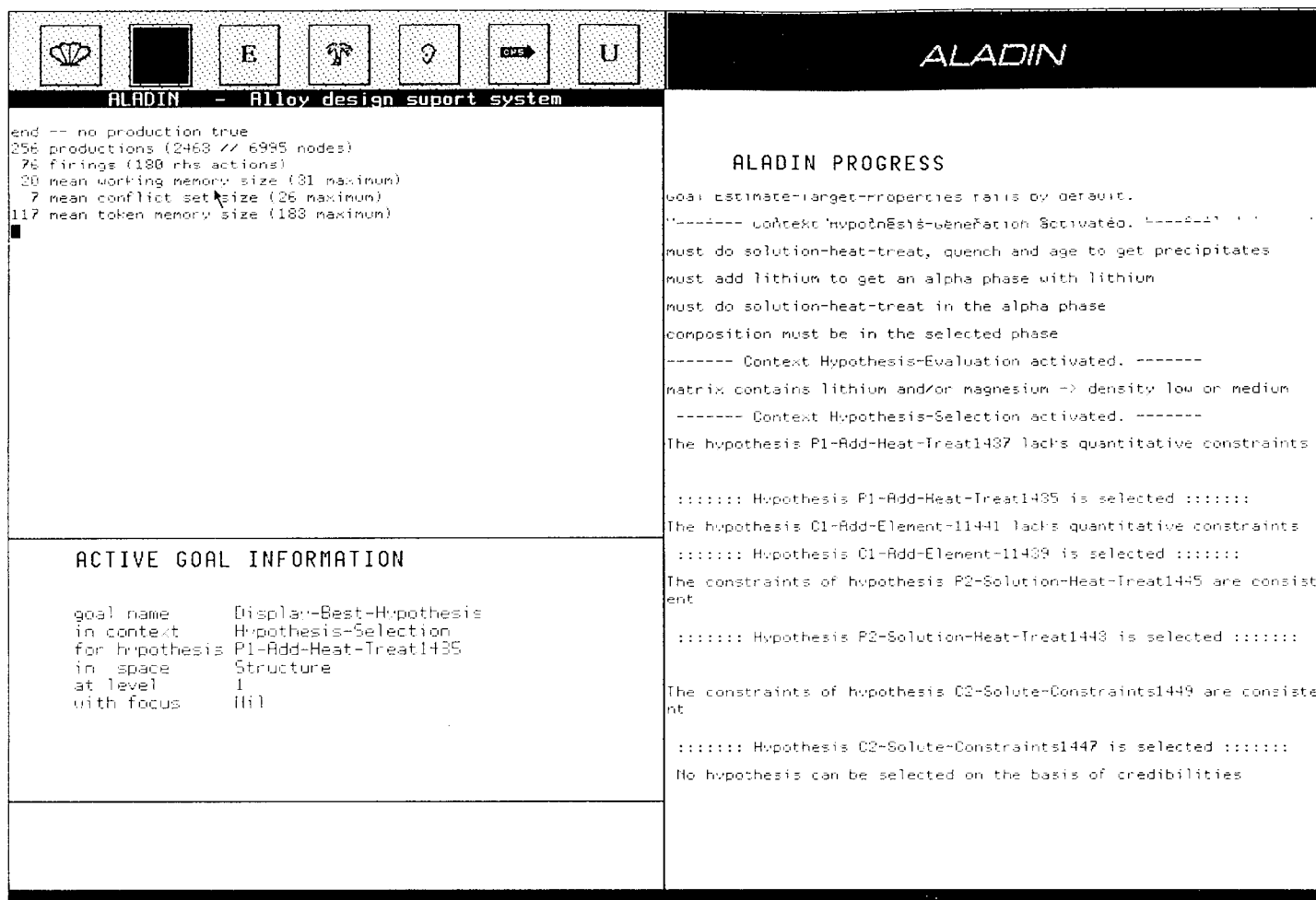


Figure 16: Quantitative hypotheses are generated

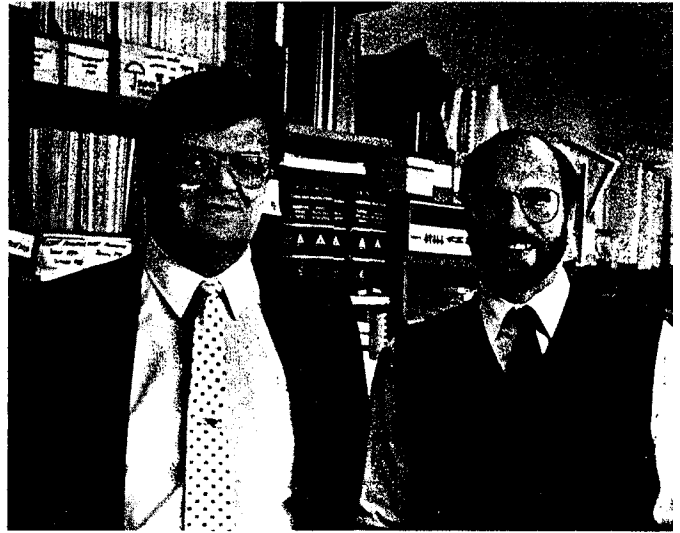
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Figure 17: Quantitative constraints are checked for consistency if present.

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