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The Metallurgical Database of Aladin -an Alloy Design System

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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, microstrocture 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 microstructme which requires a more involved representation.

2 Alloys

Alloys, when viewed from tie standpoint of their design, are interrelated and grouped in a number of different wilys. We hswc <teigtwf ft iloiiiJber of reliitiottssbips, with different inheritance semantics, to enable our schemata, to reflect tins domain organization, For example, alloys are grouped together into series and families by their

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Figure !: Alloy Groups

composition. They aie also related by the processes tf^ go into their fabrication (e.g., beat 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 axe used at various stages in the design search in older to make hypotheses and estimates. By defining classes of similar alloys they allow analogies to be dra^ii along a niimber cf different dimensions. Figure 1 depicts some of this knowledge-base stmctuie. Schemata are used to dtoSne all of flæ relations and tbstact entities Involved.

Hie 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 aie likely to produce an aMoy with desired propeities. When searchiig for trends, however, caie must be tafatolookfcrilc^to are produced in aimitar ways, have similar compositions, and were tested using identical methods. Some of these lestrictispns may be imposed by •comparing only alloys from the same aiioy-process-gioup and/or al op-example.

We will *me* ihe 2D2⁺-T⁵-sbee: aL'oy, as defied la references [6] *and* [1] to illustrate the knowledge sector station of the ALADIN & *MZ* base, five «±rattla, shown in figm» 2 - 6, *mt* required *to* describe Ms alloy.

The fefiowinf *MmmMtim m* ncpiegorted *m* figure 2: TTie aloy is a **member of the** 2xxx-T8-sfaeet gives of alloys which is further dsSised is the schema sbo^ii. m igme 3. The application of this alloy is aerospace. Several pi®p6fies s-cb is eic-ri^cr, hmw kixmD vaho and L'es se even, The rnajcr and minor alloyizig element as well *m mpukf* dfaOMOti akQg witi titwir loqpecdve I M^W ! p «cato» a are q^ified. The micTostroooie is <ksai,bed by s schema k i p w 6*

{{2024-T8-sheet **INSTANCE:** alloy **MEMBER-OF:** 2xxx-T8-sheet **ELONGATION: 6 APPLICATION: aerospace ADDinVES:** Cu nominal-percent: 4.4 class: major-alloying-element unit: weight-percent Mg nominal-percent: US class: major-alloying-element unit: weight-percent Mn... Fe.... Si... MICROSTRUCTURE: 2024-T8-Sheet-StTCt }} Figure 2: The 2024 Alloy {{2xxx-T8-sheet **INSTANCE:** process&series-group SUBSER-OR 2xxx-series-2 sheet-group T8-tonper-group **ELONGATION: 7 MODULUS: 10.6** MACHINABBLnY: B **TENSILE-YIELD-STRESS:** range:(pied(lambda(x) (and(>x51)(<x66)))> 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-graip schemata aie shown in figures 4 and 5. Information on several properties is given. Explicit property values serves as default values for membeis of the group, eg. if die 2024-T8-sheet schema lades 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 attiibute of a property is a constraint on possible values of thai property for members of the group. This constraint is coded in lisp and in tins 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 tee the fatigue is constrained to be low to medium. The meanings of linguistic variables are defined in the propeity database.

{{ sheet-group
 INSTANCE: alloy-piocess-groip
 PRODUCT:sheet
 PROCESS-MEIBODS: cast pieheai hot-roll
 cold-ioll }}

Figure 4: The Sheet Process Group

The slieet-group schema, figure 4, provides iofaomatioii ttut is commaa for sheet products, n « a dy a specific sequence of process methods mat *Is* used to make sheet **a** installations.



Figure 7: Classification of Microstructme

Although much of the heuristic knowledge about alloy design involves the microstiuctuie it is usually pooiiy 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 microstructme 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 Iks 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 urtrecrystallized 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 tree 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 microstructuie by metallurgists in the future.

In order to represent micxostracture data and rules it was necessary to develop a symbolic representation of alloy microstructure. Microstructures are classified as described by Hombogen [7] and shown in Hgure 7. Hie two main features of an alloy microstructuie 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 microstnscttjral 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 micxostractore deals with qualitative tacts and that quantitative information is typically not available.

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

FigareS: The T8-Temper

The T8-temper-group sdiema, figure 5, specifies the process methods that deteimine 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 microstructule 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: iecrystallized instance: value %;100 aspect-ratio: 2 texture: cube precipitate instance: nucrostructural-elenient phase: s-prime she: 0.1 aspect-ratio: 100 geometry: rod distribution: uniform

Figure 6: The 2024 Microstracture Representation

3 Microstnicture



Figure 8: Taxonomy of Microstructurai Elements

5.1 Structured Representation of Microstraciure

The representation of alloys (figure 1) includes the attribute MiatcmitociURE that gives the name of a schema that describes the microstructoe. In the case of 2024-T8-sheet (see figures 2 and 17) the microstructare is described in the schema 2Q24-T8-sheet-strct which Is an instance of a multi-phase-dispersioiL Microstmctures are in general classified *m* one of the categories shown in figure 7 or some sobcaiegory of than. The ability to create new subcategoiies makes die rq}iesentation flexible and extendable to other alloy families. If this representation were to be applied to steel, for example, a maiteasitic microstiucniie could be *<k£msd mad* added to the microstructure groups. The schema *shown* in figure 9 defines the attributes that are associated with a microstiuctuie group and die idjtfim to<rtta"awaq«s (fem^i the w^zitoe and and its &rwi^ ES^A+INV). Hie raw#e attribute.

{ MICROSTRUCTURE GROUP

5-A Moy-peoperty

STRUCTURH-ELE^IENIS,'

and ciement))

NUMBER OF FEASER:

(jpnd cd-^lo^p) 1J

Figure 9: Tbe-:opof iheniicrcstnicrdre bierarchy

6

32 Microstructural Elements

The microstructule is further characterized by a description of the microstructural elements that aie present Ihe 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)
EUEMENT-DENSITY:
DIMENSION:
 range: {or 0 12 3}
STRUCTURE-ELEMENTS:
 range: (all (type instance miat>stractural-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, IS 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-EIJEMENTS 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 reaystallization. The recrystallizarion-level can also be specified by the RECRYSTAIUZAHON-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: microstructuisl-element
 PHASE:
 range: (type is-a phase)
 SEE:
 ASPECT-RATIO:
 TCXTURE:
 range: (all (or copper brass S cube Goss)))))
 RBCRYSTALIJZATION-LEVEL:
 range: (or reoystalizsed partial unreaysfcallized)
 FRACTORB-IiIODe:
 StKEHGTH:}}

Figure II: Prototypical Grain

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

```
{{ GRAIN-BOUNDARY
```

```
IS-A: micK)stracturai-element
DIMENSION: 2
TYPE:
range: (or tilt twist mixed)
ANGLE:
range: (or low medium high)
PFZ-ZONE:
IMPURITY:
range: (type is-a element)
SIRENGIH:
STRESS:}}
```

Figure 12: Prototypical Grain Boundaiy

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 me 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: Ricrostractimal-element
ZS-A+INV: precipitate dispeisoid constituent
DIMENSION: 3
SIZE:
ASTCCX-EA11Q;
GBOMEXRY:
range: (or sphere rod plate oblaie-sphere)
DmUBITTOfc
range: (or number closts red regular)
FRASE:
range: (type i$-z phase)
voimmmAcnm:
STABHJIT:
```

nange: (or equilibrium meta-stable) }}

Figure 13: Prototypical Particle

MamMMmm, In the *dMwMm* sctema, figere 14, the TYPE attribute is similar to the TYPE in grain-boundary.

{{ DESLOCATION

BI-A: microstructural-clonent Ttm nge: (or edge screw mixed) DIMBN8ION: t }J

Figure 14: Dislocation

Qikm Sk-wOmm Beia«tis₉ *Tht* rtiw *siiwctim dmmm me* lepieseoted by sdiemata in figure 15, the meaning of itttteto itows the p^tenc^»b «ial>we-

{{ 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

33 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:

^M[16a] shows the as-quenched microstructure of the alloy (condition A with zero aging) where no grain boundary o* is observed although a very fine matrix 6* can be seen as a faint mottling. This 8* was presumably produced during the quench. Figure [16b] shows the microstructure in the peak-aged alloy (condition B), where the strengthening matrix 5' precipitates are seen together with coarse grain boundary 6 precipitates; these are seen as white regions surrounded by dislocations ... and a 5' precipitate-free zone (PFZ) 0.5 Jim wide which has given up its solute to the grain boundary 5."

The microstructure representations for both alloys, used in ALADIN, axe shown in figures 18 and 19. Hoiee 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 solutionizkig 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 microstracture, 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 gantitative information,

In case of FA alloy most of the lithium is in the form of either 8' precipitates inside grains or 8 particles on the grain boundary. Grain boundary has additionally precipitation free zone (PFZ) bat other characteristics of the microstructure, such as MnAl₆ dispetsoids, 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 fnicrostractujral elements allowed for the association of 8 particles and PFZ with the grain boaodaiy, a crucial feature in this microstracture.

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



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

{{ Al-3Li-0.5Mn-_pa

MEMBER-OF: experimaQtAl-Ii-Mn-series MICROSTRUCTURE: A1-3Ii-0.5Mn-pa-strc ADDmVES: U nominal-percent: 3.0 unit: wmgfA-p&zcaoi Mn nominal-percent: 0.5 unit: wd^it-pCTceirt PRCX^SS-METHODS: cast class: diTK^ soiiition-faeat'-tzcac temperature: 1020 innt; 30 streach percent-stretch: 2 т time: 48 temperature: 400 level: |»ak ctor; Mificiai}}

Figure 17; Eq>i«eiitatic» of Al-3Li-0.5Mn in Peak Aged CowMtion,

te age pim^ss roetbod is omitted in the quenched condition.

to represent my imaphable miciostnictiiie, For example let's assume that the solution teat treated alloy bas sibgrsins inside each grain *mad* tint each [sabpath consists of several cells separated by dislocation angles, to AJtdlfi, wch a stni&mt wi be fcpfesentei 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 microstnicttues can be easily represented using this method.

{{ Al-3U-0.5Mii-sht-strc MICROSIRUCTUREFOR: Al-3Ii-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 recrystalUzation-level: 100 phase: alpha-Al-Ii structure-elements: dispersoid phase: A16-Mn size: 02 probability-distribution: log-normal aspect~ratio: 3 geometry: rod length: 0.3 volume-fraction: 0.005 local-volume-fraction-distribution: log-normal missfit-strcnn: large dislocation type: mixed element-density: low grain-boundary phase: alpha-Al-Ii angle: high impurity: Na K H structure-element: dislocation type: mixed element-density: Mgh}J

ient-uensuy. Mign ja

Figure 18: Mkrastractare of Al-3Ii-0.5Mh in Quenched Condition

{{ AJ-3Li-0^Mn-pa-strc MIC3lOSTRUCrURE-POR: A1-3Ii-0.5Mn-pa STRUCTURE-ELEMENTS: grain she: length: 415 aspect-rath: 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: 02A recrystallization-level: 100 phase: alpha- Al~Ii structure-elements: precipitate phase: Al3-Li size: 0.03 probability-distribution: log-nonnal aspect-rath: 1 distribution: uniform volume-fraction: 023 local-volume-fracthn-dlstrihudon: log-normal missfit-strain: 0 dispersoM phase: A16-Mh she: 0.2 aspect-rath: 3 geometry: rod Jefl^fc; 0.3 volume-fraction: 0.005 missfit-strain: Mgh dislocation rype; mixed element-density: low

Figure W: Mcrostmctine of Al-3Ii«0.5Mh in Peak Aged Coiniition

grain-boundary phase: alpha-Al-Ii angle: high impurity: Na K pjz-zone: 025 structure-element: dislocation type: mixed element-density: high precipitate phase: Alii aspect-rath: 1 geometry: spheroid diameter: 1 volume-fraction: 0.04 missfit-strain: high }}

Figure 19, continued

4 Conclusions

This presentation accomplishes the task of representing microstnicture 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 microstnictures 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 peifonning 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 microstnictures. The general principles may also apply to the microstnicture of some non-metallic materials.

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