OVERVIEW

This document describes our annotation guidelines for marking up scientific texts in the domain of materials science with information regarding experiments on solid oxide fuel cells (SOFCs).

We follow a **frame-semantic** approach (Fillmore et al., 2006) for annotating scientific publications with the relevant information. An **experiment frame** can be thought of as a template that has to be filled with relevant information, e.g., to fill a table with information about fuel cell experiments mentioned in a collection of papers. The relevant columns in such a table are for instance ***anode_material***, ***cathode_material*** or ***fuel_used***. (For a full list, see Section 3.) In frame semantics, a frame can be evoked by some word mentioning that an experiment was conducted. This word is also called the **frame-evoking** element. In Figure 1, the word *demonstrated* is the frame-evoking element as it signals to the reader that some experiment is being described in this sentence.

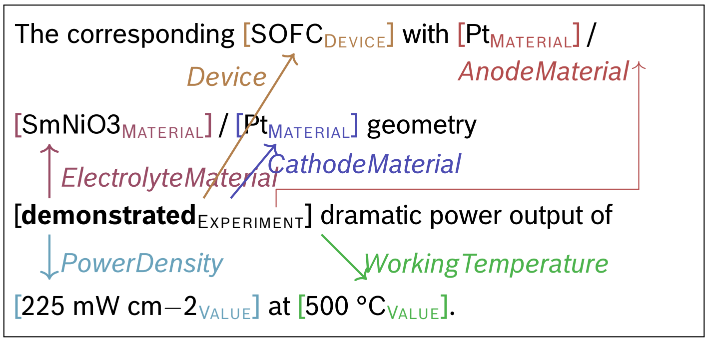

Fig. 1: Sentence describing a fuel-cell related experiment, annotated with Experiment frame information. [PMC5793538]

The relevant categories related to an experiment frame (***anode_material***, ***fuel_used*** etc.) are called the **participants** of the frame. As illustrated by Figure 1, on text, they are annotated as relations between the frame-evoking element and the span in the text mentioning the respective participant. Our annotation scheme contains several high-level (entity or concept) types for participant mentions, i.e., ***MATERIAL***, ***VALUE*** or ***DEVICE***. In addition, our annotation scheme features some additional link types that connect several experiment frame instances if they refer to the same or only slightly different experiment settings.

Our annotation scheme is tailored to the domain of fuel cell experiments. However, superclassing the fuel cell experiment frame in future work will allow for more general experiment representations, which can then in turn be adapted to other experimental domains.

The following table of contents provides an overview of our annotation scheme. In Section 6, SOFCs are explained in a nutshell.

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1 EXPERIMENT MENTIONS

As a first step, we **identify sentences that describe** a relevant solid oxide fuel cell **experiment**. Such sentences should explicitly mention at least one of the following elements:

- The material composition of the fuel cell
- The condition of operation of the fuel cell
- The type of fuel cell
- A chemico-physical property of the *whole* fuel cell

Among other things, we do **not** mark descriptions of processes, experiments unrelated to fuel cells, characterization techniques, synthesis procedures, explanations or evaluations. In this annotation pass, we do **not** mark material structure or any general material properties either.

Usually, but not necessarily, an experiment is introduced to the text by a frame-evoking verb such as *test, evaluate, measure*, or *generate*. Depending on the context, the same verb may occur as frame-evoking element or not.

We annotate the words that introduce the experiments involving fuel cells with one of these labels:

- ***current_experiment***: when **original and novel content** is introduced.
- ***previous_work***: when the sentence focuses on **specific previous work** described in detail in other sources.
- ***general_info***: when the **state of the art** of fuel cells is described, e.g., general knowledge that one could find in a textbook or in a survey.
- ***future_work***: when the authors suggest **further research topics**.

Examples

Note: For the sake of clarity, the examples in these guidelines are only partially annotated. In each section, they display exclusively the frame participants and relations that are being discussed.

- Solid oxide fuel cells (SOFCs) are based [***general_info***] on a ceramic electrolyte and work at elevated temperature between 600 and 1000 °C. [PMC4021905]
- In this report, we demonstrate [***current_experiment***] a prototypical, AAO-supported thin-film fuel cell with a bilayered electrolyte comprising a GDC film and a thin protective YSZ layer. [PMC3564701]
- Shim et al. demonstrated [***previous_work***] that a fuel cell employing a 40-nm-thick yttria-stabilized zirconia (YSZ) can generate a power density of 270 mW/cm2 at 350°C [11], while Kerman et al. demonstrated [***previous_work***] 1,037 mW/cm2 at 500°C from a 100-nm-thick YSZ-based fuel cell [12]. [PMC3564701]
- Further optimization of BEC thickness may enhance the cell performance, which could lead [***future_work***] to wider potential applications of AAO supporting TF-SOFCs as high-efficiency power sources. [PMC4578433]
- Citric acid ($99^{+}\%$, Alfa Aesar), in a 2:1 molar ratio to the metal ions in the final product, was added and heated till a solution was formed. *[synthesis route: no annotations here]* [PMC5075869]
- In general, a scan rate of 2Hz and a resolution of 512$\times$512 pixels over a scan area of 1$\times$1 μm^2 2were chosen. *[characterization technique: no annotations here]* [PMC6158676]
- X-ray diffraction of $SrFe_0{\cdot}_9{-}xCuxNb_0{\cdot}_1O_3{-}\delta$ (x = 0–0.4) showed that it exhibited a single phase cubic perovskite structure (SG: Pm-3m) for all compounds. *[Experiment not about SOFC: no annotations here]* [PMC5075869]

- La_2O_3, $SrCO_3$ and Co powders (all Sigma-Aldrich, 99.995%) were individually dissolved in nitric acid, mixed inappropriate ratios and citric acid (TraceSELECT, 99.9998%) was added for chelation. *[synthesis route: no annotations here]* [PMC6158676]
- The electrolyte support cell used in this study was prepared through a tape casting process, with the outer two layers having pore formers. *[processing: no annotations here]* [PMC5075869]

2 PARTICIPANT TYPES

This section describes the high-level **entity or concept types** that are used to mark the spans in the text referring to the participants of an experiment. In order to keep the amount of required annotation feasible, but also provide training data for these types independent of the frame mentions, we decide to mark all mentions of instances of these types that occur within or in the neighbourhood of sentences actually describing a fuel cell experiment. We use a loose definition of neighbourhood, including the paragraph or, if paragraph boundaries are unclear, the surrounding sentences. Annotators are asked to apply their own common sense to define the "relevant neighborhood" for a sentence.

2.1 *MATERIAL*

We use the type ***MATERIAL*** to annotate text spans referring to materials, elements or substances that are mentioned as a participant in a fuel cell experiment. (For a list of such participants, see Section 3.) These participants may be specified by a particular material composition formula (e.g. $La_{0.75}Sr_{0.25}Cr_{0.5}Mn_{0.5}O_3$) or, at the other end of the spectrum, just by a mention of the general class of materials such as *oxides* or *hydrocarbons*. If a cell component (e.g., an electrode) is composed of multiple materials, we annotate all of them, if possible as a single span. References to previous mentions of the material as in *material, this, new anode* etc. can also be annotated as spans of type ***MATERIAL***. (In this case, if the mention is not informative on its own, a ***coreference*** link should be added as described in Section 4.2.) Adjectives relative to the material are included in the annotation only if they are necessary to distinguish between different materials that may have the same composition.

Examples

In the following examples, all underlined spans are marked as ***MATERIAL***.

- Gadolinium-doped ceria (GDC) has been considered as a promising electrolyte material due to its excellent oxygen ion conductivity at low temperatures. [PMC3564701]
- A low temperature active cathode (like LaSrCoFe-oxide or SmSrCo-oxide) can be used, together with an interlayer against diffusion or reaction for long term stability. [PMC4021905]
- They run not only on hydrogen, but also on widely available hydrocarbon fuels. [PMC4222441]
- The cells consisted of Ni-YSZ functional anode, YSZ electrolyte and (La0.8Sr0.2)0.95MnO3-δ (LSM)-YSZ cathode prepared in sequence on the substrate by dip-coating and sintering. [PMC4313086]
- The cell stacks composed of Ce0.9Gd0.1O1.95 porous electrolyte and La1−xSrxMnO3 (x = 0.15, and 0.5) composite electrode were investigated by Werchmeister et al. [80]. [PMC3730159]

2.2 *VALUE*

We annotate numerical values and their respective units with the type ***VALUE***. As illustrated by the examples below, we include both the numbers and the units in the annotation span. In addition, we include comparative specifiers like *more than, between* etc.

Examples

In the following example, all underlined spans are marked as ***VALUE***.

- The single-phase SP parent material Ba0.5Sr0.5(Co0.8Fe0.2)O3−δ itself is an MIEC and effective SOFC cathode that displays a range of ASR values from 0.03 to 10 Ω·cm2 at 650 °C. [PMC3793895]

2.3 *DEVICE*

The type ***DEVICE*** is used to mark mentions of the device used in the fuel cell experiment. We do not include any modifiers such as adjectives in the annotation span.[1]

Examples

- The corresponding SOFC with Pt/SmNiO3/Pt geometry demonstrated dramatic power output of 225 mW cm-2 at 500°C. [PMC5793538]

[1] This annotation is not very informative on its own at the moment. We nevertheless add the reference to the relevant SOFC devices as in future work, we plan to link the ***DEVICE*** mention spans to their finer-grained types defined in a domain ontology, which provide information about the type or class of fuel cell w.r.t. the class of electrolyte materials (SOFC, PEM...), the geometry (planar, tubular...) and the range of operating temperatures (high, intermediate...).

3 EXPERIMENT PARTICIPANTS (RELATIONS)

The relations explained in this section are used to indicate the participants of an experiment frame. In order to group the various materials, values etc. into experiments, we connect them to the word in the text that indicates that an experiment was conducted, i.e., the frame-evoking element. All of these relations have their **starting point** at the frame-evoking element and their **end point** at the respective participant.

An experiment participant should always be connected to the closest frame-evoking element, which should be located in the same sentence and preferably in the same clause of the participant. If the information about the participants of an experiment is spread over multiple sentences, please connect the participant mention to the closest experiment-evoking verb and then group these verbs by connecting the frame-evoking elements with ***same_experiment***.

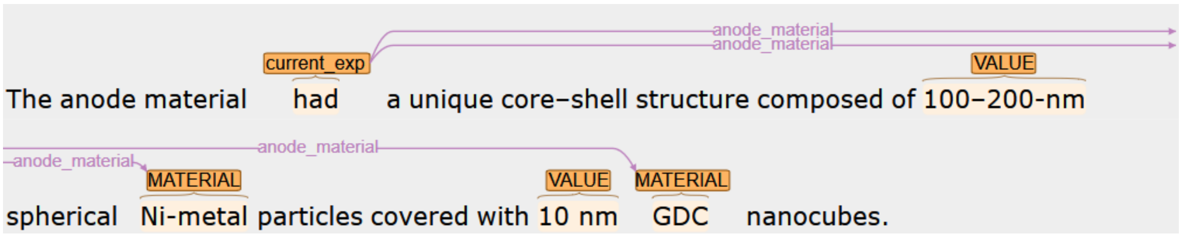
3.1 *anode_material*

This relation is used to mark connections between the frame-evoking element and the material that makes up the anode.

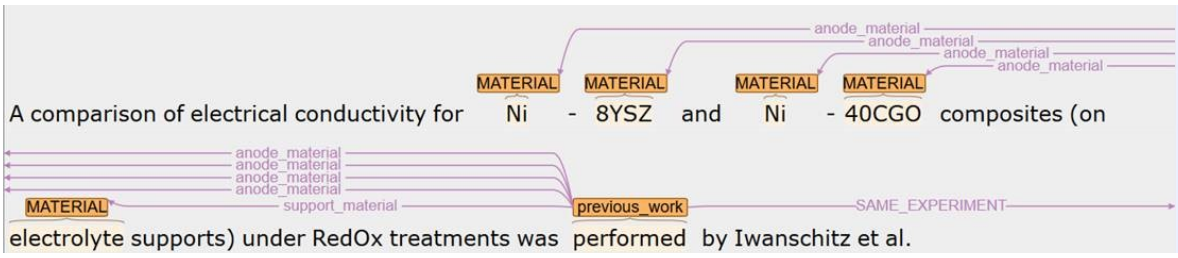
As a convention, we will always annotate the fuel electrode as anode material (even in case of electrolytic cells). We annotate as anode materials also the ion conductive material in a composite anode even if the electrolyte is made of the same material. For example, if there are two materials present in the anode, we annotate them both as ***anode_material***, even if one of them is also the electrolyte material.

See 6.3 for more information about anodes in solid oxide fuel cells.

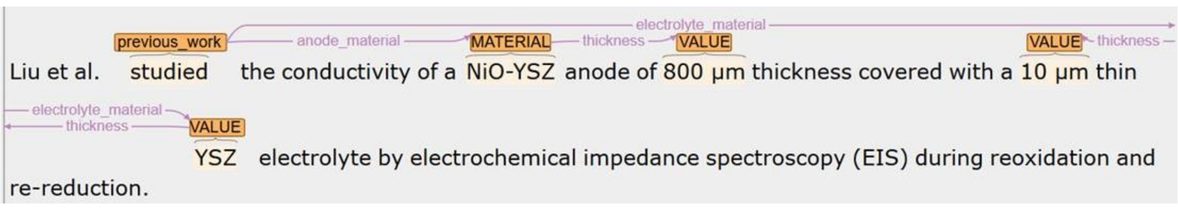
Examples



[PMC4663492]



[PMC4021905]



[PMC4021905]

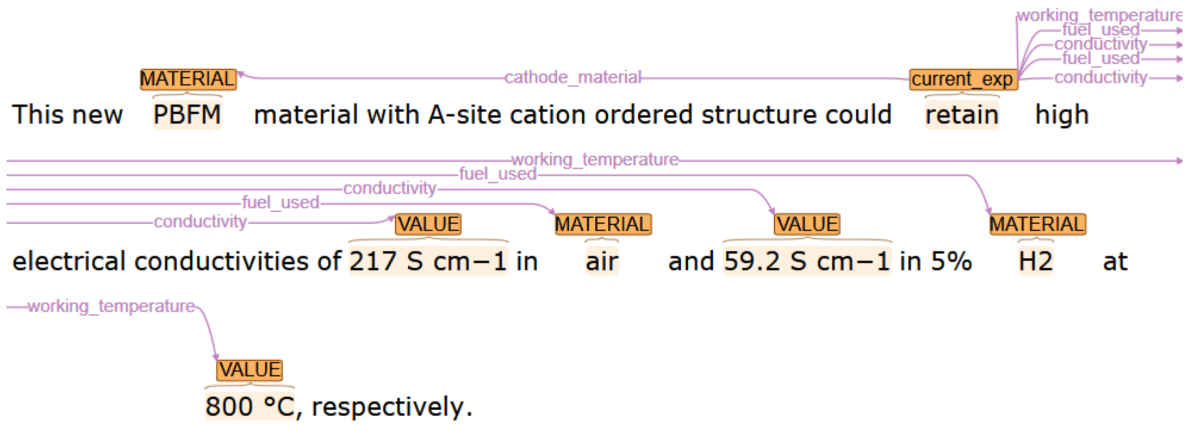
3.2 *cathode_material*

This relation is used to connect the frame-evoking element and the material that makes up the cathode.

As a convention, we will always annotate the oxygen electrode as a cathode material (even in case of electrolytic cells). We annotate as cathode materials also the ion conductive material in a composite cathode even if the electrolyte is made of the same material. For example, if there are two materials present in the cathode, we annotate them both as ***cathode_material***, even if one of them is also the electrolyte material.

See Section 6.2 for more information about cathodes in solid oxide fuel cells.

Example



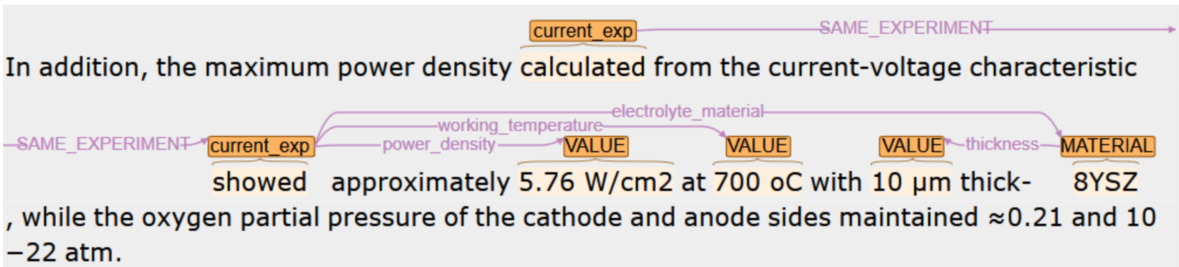
[PMC4673446]

3.3 *electrolyte_material*

This relation connects the frame-evoking element and the material that makes up the electrolyte.

Electrolytes are briefly discussed in section 6.4.

Example



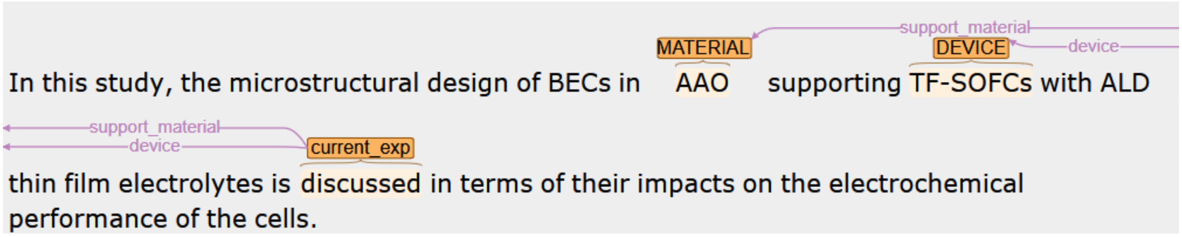
[PMC4698742]

3.4 *support_material*

This relation connects the frame-evoking element and the material that makes up the support of the cell.

For more information, see Section 6.7.

Example

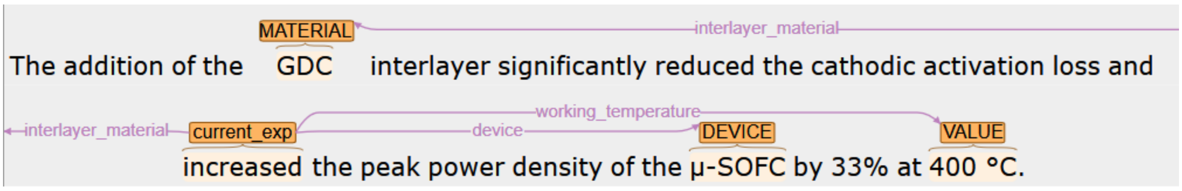


[PMC4578433]

3.5 *interlayer_material*

This relation connects the frame-evoking element with a material used as interlayer or buffer layer in a SOFC.

Example

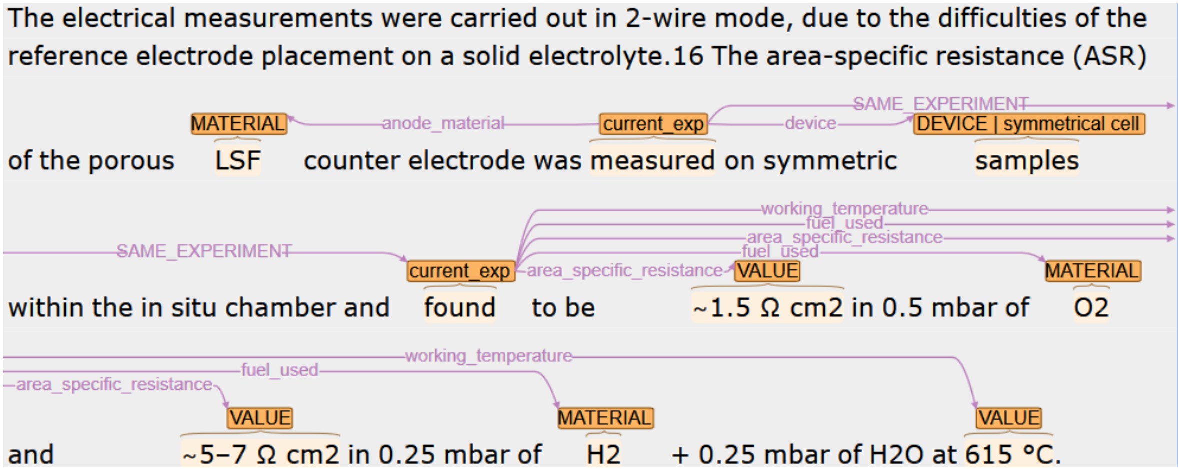


[PMC4770875]

3.6 *fuel_used*

This relation connects the frame-evoking element and the chemical composition or the class of a fuel or the oxidant species (indicated as a material).

Example



[PMC4735809]

3.7 *device*

This relation is used to connect the frame-evoking element and the device tested in this experiment.

Example See examples in Sections 3.5 and 3.6.

3.8 *degradation_rate*

This relation connects the frame-evoking element with the degradation rate of the cell, which can be also expressed as a percentage.

Example Adversely, cobaltite-based cathodes were shown to be prone to significant long-term degradation of ~0.05% per hour [20].

[PMC6523084]

3.9 *power_density*

This relation connects the frame-evoking element with the values of the (maximum/peak) power density obtained from a device.

Example The corresponding SOFC with Pt / SmNiO3 / Pt geometry demonstrated dramatic power output of 225 mW cm−2 at 500 °C [16].

[PMC5793538]

3.10 *resistance*

This relation connects the frame-evoking element to the mention of the electrical resistance of a cell or cell component. In SOFC experiments, the ***resistance*** is usually expressed in area specific units: $\Omega\,\mathrm{cm}^2$. Ohmic resistance and polarization resistance can be distinguished via the corresponding entries in the knowledge base.

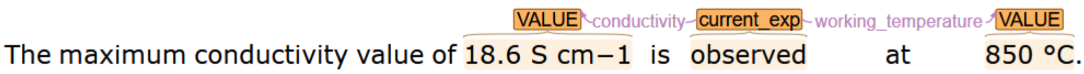
Example Moreover, the very high electrode activity of the LSC film required a different type of counter electrode: porous LSC thin films with a polarization resistance of 0.1–0.2 Ω cm2 at 600 °C in air (at least 1 order of magnitude below the working electrode ASR)12 were fabricated via PLD by decreasing the deposition temperature and increasing the chamber pressure to 450 °C and 0.4 mbar, respectively.

[PMC4735809]

3.11 *conductivity*

This relation connects the frame-evoking element to the mention of the electrical conductivity of a certain cell or cell component. Electronic and ionic conductivites can be distinguished via the corresponding entries in the knowledge base.

Example

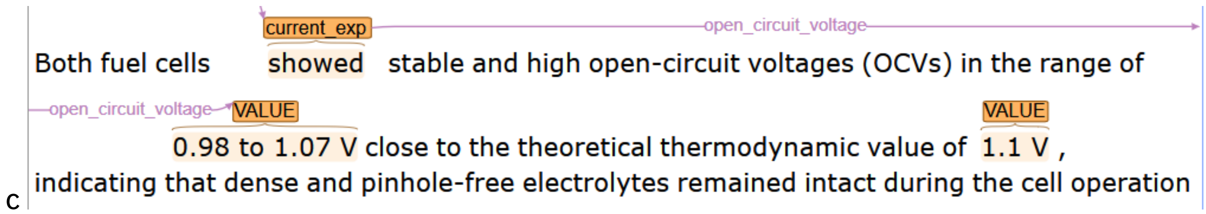


[PMC6632008]

3.12 *open_circuit_voltage*

This relation connects the frame-evoking element and the value of the open circuit voltage (OCV) obtained from a device.

Example

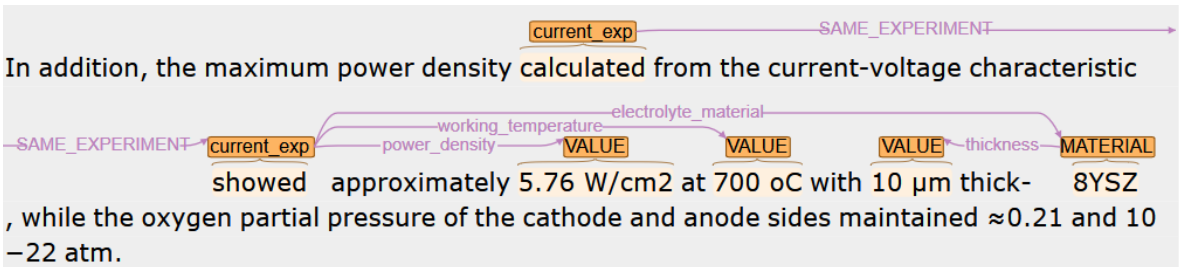


[PMC4770875]

3.13 *working_temperature*

This relation connects the frame-evoking element with the value of the temperature at which the cell is operated or at which a certain experiment has been performed. If the temperature is expressed as a range (e.g., "between 700 and 800 °C"), this ***VALUE*** is marked as a single span. If a sentence mentions several experiments with differing temperatures, but only one frame-evoking element can be identified, simply link all temperature values to this element. For example: "It can be **seen**[EXPERIMENT] that the electrode polarization resistances in air are 0.027 Ωcm^2, 0.11 Ωcm^2, and 0.88 Ωcm^2 at 800 °C[***working_temperature***], 700 °C[***working_temperature***] and 600 °C[***working_temperature***], respectively." [PMC4673446] Note that in this case, each of the values is annotated as a separate link as they do not correspond to a range of values but to different experiments.

Example



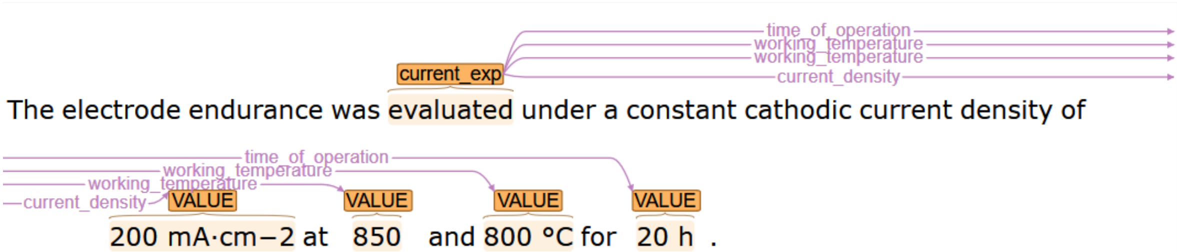
[PMC4698742]

BOSCH

3.14 *time_of_operation*

This relation connects the frame-evoking element with the value of the duration of an experiment. The duration of an experiment can be expressed in hours or as a number of RedOx cycles.

Example

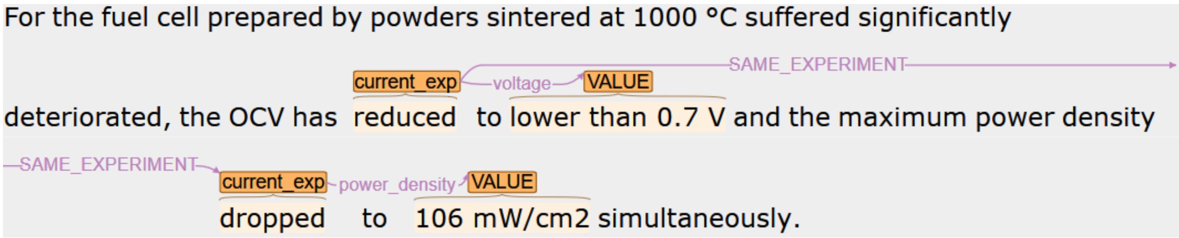


[PMC6632008]

3.15 *voltage*

This relation connects the frame-evoking element with the value of the voltage at which a cell was operated. Not to be confused with ***open_circuit_voltage*** (see Section 3.12).

Example



[PMC6517467]

3.16 *current_density*

This relation connects the frame-evoking element with the value of the current density of that experimental setup.

Example

See example in Section 3.14.

4 ADDITIONAL ANNOTATIONS

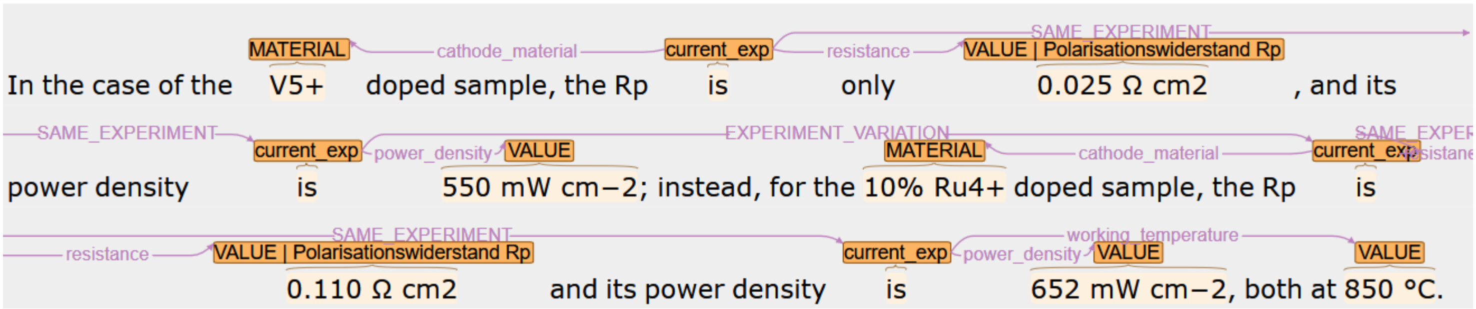
We here describe several relations that are not part of the Experiment frame.

4.1 *same_experiment* and *experiment_variation*

The relations described in Section 3 all assume that the frame-evoking elements occurs in the same sentence as the participants of the frame. Very often, however, the description of an experiment is spread over several sentences. Annotators are then asked to link the frame participants to the closest frame-evoking element, which usually is in the same sentence. The relations explained here are used to connect several frame-evoking elements that describe the exact same experiment or variations of the experimental settings explained above. While at times it may be difficult to differentiate them, we distinguish the following two cases:

- ***same_experiment***: This relation connects words introducing a fuel cell experiment with a following frame-evoking element indicating more experimental information on the same cell with the same experimental conditions. Sometimes the frame-evoking elements of this kind have a meaning of further or deeper investigation or explanation, e.g. *can be seen*, *exhibit* etc.
- ***experiment_variation***: This relation connects a frame-evoking element with another frame-evoking element indicating an experiment on the same cell, but with further specifications or slightly different operating conditions. It can also relate two frame-evoking elements that refer to two measurements performed on *different* materials/cells, but at the *same* experimental conditions. Often the frame evoking elements of a subexperiment convey an idea of comparison, e.g., *increase* or *reach*.

Example



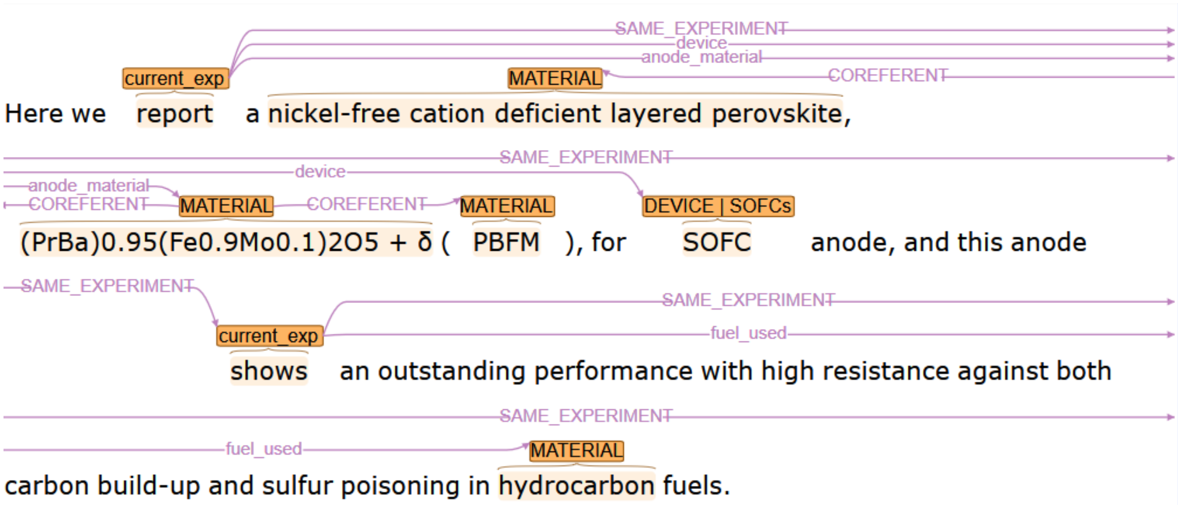
[PMC6632008]

In the above example, ***same_experiment*** was used to connect the experiment descriptions if the participants, i.e., the experimental settings and measurements, should be grouped together. Another example is given in Section 4.2.

4.2 *coreference*

This relation connects the mention of a frame participant with an earlier mention of the same entity. We do not aim at a comprehensive coreference annotation, but use this only if the mention of a frame participant is uninformative, e.g., if pronouns or abbreviations are used. In this case, we link it to an earlier informative mention. (This procedure will not allow us to evaluate coreference in the domain of materials science, but using these annotations, we can simulate a setting where perfect coreference information would be available for frame participants in our experiments.)

Example

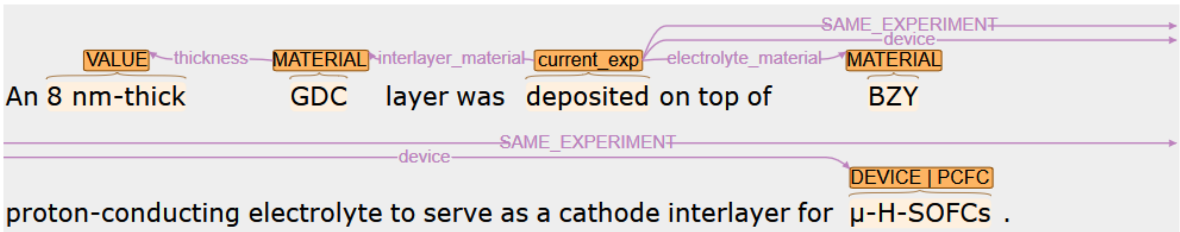


[PMC4673446]

4.3 *thickness*

This relation can be used to give further information on a material used for composing cell. It relates the ***MATERIAL*** mention with the mention of the ***VALUE*** expressing the material's **thickness**.

Example



[PMC4770875]

5 WHAT IF...

This section describes some questions that arise during annotation and our respective decisions.

5.1 ...multiple parameter settings are described within one experiment frame?

Sometimes, authors condense their text by reporting several experiments or experiment variations within the same sentence. Usually, this means that several parameter settings that were tested are being reported at the same time, as illustrated by the example below. While it would be desirable to induce multiple Experiment frame instances in this case, it is difficult to annotate and also a challenge to any state-of-the-art machine learning system. From a use case point of view, if a system is able to extract such a "series" of experiments correctly, recognizing the respective participants and their types correctly, this would already be very valuable. We hence leave the step of disentangling these multiple-experiment mentions to future work. Note that this means that we allow frame participants to occur multiple times in our frame instances.

Examples

- It can be **seen**[EXPERIMENT] that the electrode polarization resistances in air are 0.027 Ω**cm**^{2}[***resistance***], 0.11 Ω**cm**^{2}[***resistance***], and 0.88 Ω**cm**^{2}[***resistance***] at 800 °C[***working_temperature***], 700 °C[***working_temperature***] and 600 °C[***working_temperature***], respectively." [PMC4673446]

5.2 ...it is unclear whether a verb is a frame-evoking element?

Sometimes experimental mentions that should be marked are not clearly distinguishable from verbs that should be excluded from the annotation. The criterion that we use in this case is to mark exclusively mentions that can be immediately identified as complying to the indications in Section 1, without overthinking.

5.3 ...an experiment is described by more than one sentence?

Our annotation scheme is not tied to sentences. Hence, the participant mentions related to one frame-evoking element may also occur in a neighboring (usually following) sentence. If there is a new frame-evoking element, we link the participant mentions to that as described in Section 4.1. If there is no new frame-evoking element, we simply link the participant mentions to the frame-evoking element in the previous sentence.

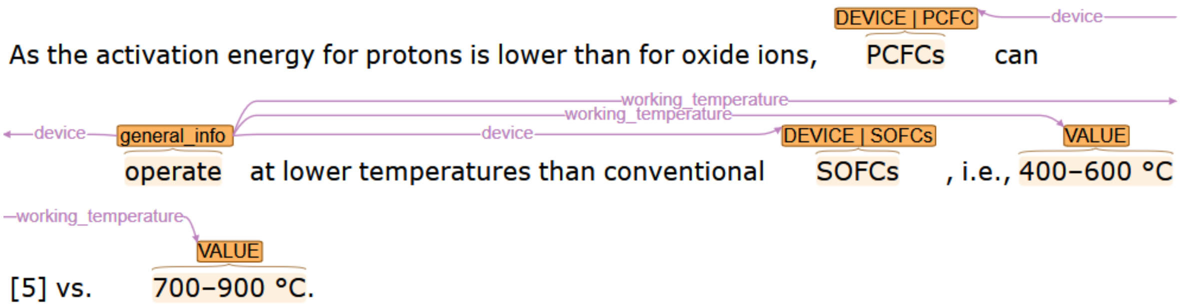
5.4 ...the participants of an experiments could be linked to different frame-evoking elements present in the same sentence?

When there are more frame-evoking elements in the same sentence, the participants should be linked to the one that is a main verb and it is situated in the same clause of the participants.

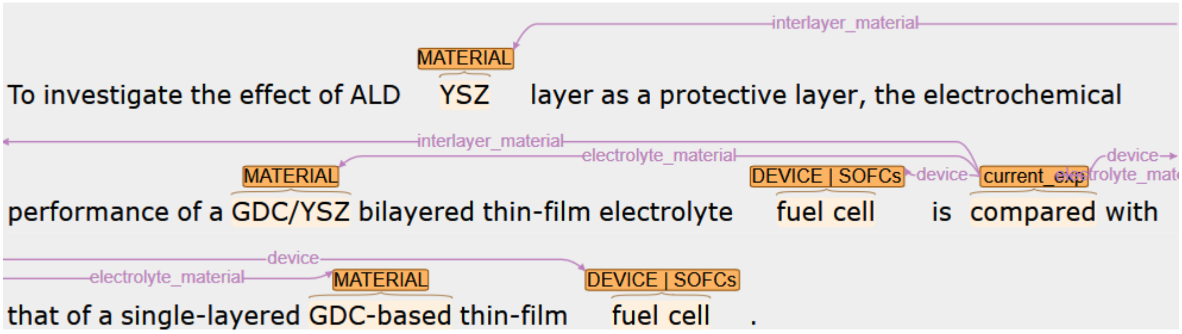
5.5 ...two experiments are compared using only one verb?

When two or more experiments are compared, sometimes a sentence with only one frame-evoking element is used. In this case, we mark all the participants, even if they are mutually exclusive. Similarly as in Section 5.1, we leave the disentangling to future work.

Examples



[PMC5848893]



[PMC3564701]

6 SOLID OXIDE FUEL CELLS 101

This section is intended as a quick reference that aims to provide a - quite simplistic - overview on the solid oxide fuel cell technology. It addresses the terms and notions that can be more frequently encountered in the domain-specific scientific literature.

6.1 Solid oxide fuel cell

A fuel cell is a device that produces electricity by oxidation of a fuel (6.6) in what is called a redox reduction. Typically, a fuel cell is composed of two electrodes and an electrolyte that separates them. In a solid oxide fuel cell (SOFC), the electrolyte is in the solid state and is made of various ceramic materials containing oxygen, the oxides. At the cathode of an SOFC, oxygen molecules are adsorbed, split and reduced (they gain electrons) (6.2). Then, they migrate to the anode through the electrolyte (6.4). At the anode the fuel is adsorbed, split, oxidized (it loses electrons) and it combines with the oxygen ions coming from the electrolyte (6.3). In order to allow the reaction and the motion of charge carriers, the operating temperature must be high enough. Within a stack, many fuel cells are connected through an interconnecting material (6.5). The advantage of the SOFCs is a very high energy efficiency, their disadvantages are caused by the high operating temperature (6.12) and include long start-up times, degradation, high material costs.

6.2 Cathode

In an SOFC, the cathode is the oxygen electrode, where oxygen molecules are adsorbed, split and reduced (they gain electrons). After this, they migrate to the electrolyte. The cathode should therefore exhibit a catalytic effect, reducing the activation energy of the oxygen reduction reaction (ORR). In addition to this, it should be electronically conductive and porous, to allow the gaseous oxygen to arrive at the reaction site. Ideally, it should also be ionically conductive, enabling the migration of oxygen ions the electrolyte, in which case the material is a mixed ionic electronic conductor (MIEC). Otherwise, the oxygen reduction reaction can only happen at the triple phase boundary (TPB), i.e. the interface between the cathode material, which is electronically conductive, the electrolyte, which is ionically conductive, and a pore, which allows the flow of the oxygen gas.

6.3 Anode

In an SOFC, the anode is the fuel electrode, where fuel molecules are adsorbed, split and oxidized (they lose electrons). Then they combine with the oxygen coming from the cathode via the electrolyte and form a byproduct. The anode must be electronically and ionically conductive, porous and act as a catalyst. Moreover, it should be resistant to deactivation that could be caused by unwanted adsorption of gas atoms on the surface.

6.4 Electrolyte

In an SOFC, the electrolyte separates the anode and the cathode and must be ionically conductive, as the negatively charged oxygen atoms (anions) diffuse through the electrolyte from the cathode to the anode, but it must not conduct electrons. There are also types of fuel cells, called proton conducting fuel cells, in which positively charged ions (cations) diffuse from the anode to the cathode instead. The most common solid oxides used as electrolyte materials are ytria-supported zirconia (YSZ) and gadolinium-doped ceria (GDC).

6.5 Interconnect

The interconnect connects the cells belonging to the same stack. It is electron conductive and it can be a ceramic material or a metal. In the latter case, the diffusion of chromium from the interconnect to other cell components is a common issue. The interconnect should be stable at high temperature both in reducing and oxidizing atmosphere.

6.6 Fuel

The fuel of an SOFC is the educt at the anode side and can either be pure hydrogen or a carbon based fuel, such as hydrocarbons or carbon monoxide. The byproduct is water in the first case, mostly carbon dioxide in the second. Even if an SOFC is fueled with hydrocarbons, its environmental impact is lower than conventional combustion engines, because its efficiency is higher. However, hydrocarbons fuel may cause deposition of carbon on the anode, leading to lower power output.

6.7 Support

The support material provides mechanical support to the cell. An SOFC can be anode, cathode, electrolyte or metal supported. The support should be stable at high temperatures and, if possible, cheap.

6.8 Thermal expansion coefficient (TEC)

This material property indicates the relative expansion of a material with increasing temperature measured in millionths over Kelvin. It is crucial that in an SOFC, the utilized materials have compatible TEC, to ensure mechanical stability.

6.9 Power Density

This properties indicates how much power per unit of area is generated in a fuel cell. It is measured in $\mathrm{W\,cm^{-2}}$ and depends on the temperature, the materials and the fuel used. It is a key quantity for the evaluation of the cell performance.

6.10 Electrical Resistance

The total electrical resistance per unit area of an SOFC has two components: ohmic resistance and polarization resistance. In common SOFCs materials, they both increase when temperature decreases.

The **ohmic resistance** indicates how difficult it is to move charge carriers inside a material. It corresponds to the inverse of the conductivity multiplied by the material thickness.

The **polarization resistance** is an electric property of an interface between two materials and is measured in $\Omega\,\mathrm{cm^2}$. It is related to the oxygen reduction reaction rate (the electrocatalytic activity) and the oxygen conductivity inside a material. A high polarization resistance means that the oxygen reduction reaction happens slowly and oxygen vacancies cannot easily diffuse and cross the interface. Therefore charge accumulates at the electrode surface, polarizing it.

The terms *Area Specific Resistance (ASR)* and *Polarization Resistance* are often used interchangeably.

6.11 Open Circuit Voltage (OCV)

The open circuit voltages corresponds to the voltage generated by the redox reaction, which can be measured in a cell without any electrical current flow. In the ideal case, its value should approach the theoretical one derived by the Nernst equation, but is commonly lower due to losses. The OCV typically decreases with increasing temperature.

6.12 Operating Temperature

There are different types of SOFCs that typically work at different temperatures: Intermediate-temperature SOFCs usually operate between 650 and 800°C and high-temperature SOFCs between 800°C and 1000°C .

While it is generally desirable to decrease operating temperatures due to long start-up times and stability issues of the materials, the conductivity of the cell components and the reaction rates typically decrease with increasing temperature. Designing high performance SOFCs that work at intermediate temperatures is therefore a field of ongoing research.

References

Fillmore, C. J. et al. (2006). Frame semantics. Cognitive linguistics: Basic readings, 34:373–400.