Plasma-MDS – A metadata schema for applied plasma science and plasma medicine

Steffen Franke¹, Lucian Paulet¹, Jan Schäfer¹, Deborah O’Connell², Markus M. Becker¹

¹Leibniz Institute for Plasma Science and Technology (INP), Felix-Hausdorff-Str. 2, 17489 Greifswald, Germany
²York Plasma Institute, Department of Physics, University of York, Heslington, York, YO10 5DD, U.K

E-mail: markus.becker@inp-greifswald.de

July 19, 2019

Abstract. A metadata schema, named Plasma-MDS, is introduced to support research data management in applied plasma science and plasma medicine. Plasma-MDS is suitable to facilitate the publication of research data following FAIR principles in domain-specific repositories and with this the reuse of research data for data driven plasma science. The metadata schema takes into account common features of research in applied plasma science and plasma medicine. This is expressed by the choice of basic schema elements, namely “plasma.source”, “plasma.medium”, and “plasma.target”. These schema elements reflect the fact that most research data in the scientific domain under consideration refer to a plasma source that is operated in a certain medium and usually acting on a specific target. This novel metadata schema is first applied for the annotation of datasets published in INPTDAT—the interdisciplinary data platform for plasma technology.

Keywords: Research Data Management, Metadata Schema, Plasma-MDS, INPTDAT

1. Introduction

The rapid progress in data science methods for machine-based analysis of big data provides enormous potential for new data driven sciences and the development and optimization of innovative technologies. Recently, first approaches have been published that use machine learning methods for simulation, diagnostics and control of technological plasmas, see [1,2] and references therein. The potential of data driven science can only be fully explored if research data is findable, accessible, interoperable and reusable (FAIR) for both humans and computers. This requirement has recently been pinpointed by the FAIR data principles [3–5] (cf. table 1). The minimum requirements for “fair” research data are that the data is made public and that it is well documented by additional metadata. The quality of metadata plays a key role for the degree of “fairness”. Once the (meta)data is registered or indexed in a searchable
resource with a unique and persistent identifier, the machine-readable metadata should contain information on how the data can be accessed, how it can interoperate with applications or workflows for analysis, storage and processing, and in which context it can be reused, i.e., detailed information on the scope of the data, lab conditions, process parameters, etc. [5].

Table 1. The FAIR Guiding Principles according to Wilkinson et al. [3].

| To be Findable                                      |
|----------------------------------------------------|
| F1 (meta)data are assigned a globally unique and persistent identifier |
| F2 data are described with rich metadata (defined by R1 below)          |
| F3 metadata clearly and explicitly include the identifier of the data it describes |
| F4 (meta)data are registered or indexed in a searchable resource        |

| To be Accessible                                      |
|------------------------------------------------------|
| A1 (meta)data are retrievable by their identifier using a standardized communications protocol |
| A1.1 the protocol is open, free, and universally implementable |
| A1.2 the protocol allows for an authentication and authorization procedure, where necessary |
| A2 metadata are accessible, even when the data are no longer available |

| To be Interoperable                                   |
|------------------------------------------------------|
| I1 (meta)data use a formal, accessible, shared, and broadly applicable language for knowledge representation |
| I2 (meta)data use vocabularies that follow FAIR principles |
| I3 (meta)data include qualified references to other (meta)data |

| To be Reusable                                       |
|------------------------------------------------------|
| R1 meta(data) are richly described with a plurality of accurate and relevant attributes |
| R1.1 (meta)data are released with a clear and accessible data usage license |
| R1.2 (meta)data are associated with detailed provenance |
| R1.3 (meta)data meet domain-relevant community standards |

In many scientific disciplines established scope-specific metadata standards exist that are recognised and broadly used by the community. Dictionaries of disciplinary metadata standards are provided by the Digital Curation Centre (DCC) [6] and the Research Data Alliance (RDA) [7], for example.

Although there are a number of databases which are relevant for plasma physics research, e.g. the NIST Atomic Spectra Database [8], the LXcat database [9][10] and Quantemol-DB [11][12], there is no database that is specifically designed for the curation of research data from applied plasma physics. This hinders the reuse of and access to data in this specific domain (cf. table 1). Furthermore, there are no metadata standards to describe this kind of research data efficiently. However, domain-specific metadata are required to enable findability, interoperability, and reusability of data (cf. table 1). The present manuscript suggests a metadata schema for research data in applied plasma
Plasma-MDS aims to be a starting point for the development of an established standard for the documentation of digital data obtained from research in the area of plasma technology. With this, it supports recent attempts to enable “a new era of plasma science and technology research and development” \cite{13} by data-driven discovery in plasma science and provides a basis for participation of the community in comprehensive developments with respect to research data management like for example the European Open Science Cloud (EOSC) \cite{14} and the National Research Data Infrastructure (NFDI) in Germany \cite{15}.

The manuscript is organized as follows. In section 2 the metadata schema Plasma-MDS is introduced. Then, its practical application is demonstrated using two examples in section 3 and in section 4 the benefits of Plasma-MDS with respect to the FAIR data principles are discussed. Section 5 summarizes the work and outlines necessary future steps.

2. Plasma metadata schema (Plasma-MDS)

Metadata represent extra information attached to data that allows people and automated processes to find, access and ultimately reuse data. Among others, Dublin Core \cite{16} and DataCite Metadata Schema \cite{17} represent fundamental metadata schemata that are widely used for the collection of general metadata of digital objects such as title, publication year, and permanent identifier. However, the “degree of fairness” of public research data (cf. table \ref{tab1}) can dramatically be enhanced by adding additional domain-specific metadata. The new metadata schema Plasma-MDS can be used as an extension to general metadata schemata in applied plasma physics and plasma medicine. It comprises various metadata fields related to the plasma source, the plasma medium and the plasma target. Furthermore, metadata fields related to the applied diagnostics and the published resource are included. Here, diagnostics also aims to cover possibly applied modelling and simulation methods.

Only the diagnostics and resource metadata fields are designed to be mandatory. This is because in one study the focus might be on the diagnostics of a certain target, while in another the simulation of a plasma source without inclusion of any target might be of interest. However, it is strongly suggested to complete as many metadata fields as possible in order to ensure a high level of “fairness” of the data. Furthermore, there is no controlled vocabulary so far to provide maximum flexibility in the definition of metadata. It is intended to review the plasma metadata schema after an initial phase of growing usage and to evaluate the establishment of a community standard including controlled vocabularies.

The metadata schema definition follows the nomenclature “schema.element.qualifier”. The motivation for the main schema elements “source”, “medium”, and “target” lies in the fact that almost every scientific result in applied plasma physics refers to a plasma source (e.g. atmospheric pressure plasma jet) which is operated in a medium (e.g. ar-
gon) and acting on a target (e.g. biological tissue). Furthermore, applied plasma physics utilizes a variety of diagnostic methods (e.g. laser absorption spectroscopy) and there are numerous scientific papers which concentrate on specific aspects of the plasma diagnostics rather than on a certain plasma (source, medium, and target). Therefore, plasma diagnostics is considered as a separate schema element, namely “plasma.diagnostics”. Finally, the schema element “plasma.resource” specifies details of the digital data object.

Plasma-MDS distinguishes the three different field types “controlled list”, “term list”, and “free text”. Controlled list means that pre-defined categories are available for selection. Term lists are defined as compilations of keywords generated on-the-fly from terms already describing the respective element in a specific data repository using Plasma-MDS. They are used whenever the establishment of controlled lists maintained by the community is an option in the long-term perspective. On the other hand, free text fields aim to give more detailed information on the respective element that cannot be represented by well-defined terms.

2.1. Plasma source

The schema element “plasma.source” has five qualifiers. First, “plasma.source.name” designates the plasma source. Several plasma source names can be entered here, if the data are related to several plasma sources. Furthermore it might be helpful to give not only the trademark name (e.g. “kINPen® MED”, which is a certain plasma source developed at the INP) but to name also the type of the plasma source (e.g. “HF plasma jet”, which indicates that the “kINPen® MED” is a high frequency plasma jet). This should increase findability of datasets including sought-for plasma sources. Before adding a new plasma source name to a database using Plasma-MDS as metadata schema, it should be verified that this value is not already given taking care for differing notations.

Next, the qualifier “plasma.source.application” informs about the application area the plasma source and the dataset are related to. Several terms can be given here describing different aspects of the application, for example plasma medicine or surface treatment. The first term identifies the dataset to be related to the topic plasma medicine, whereas the second term describes the more technical aspect of surface treatment in contrast, e.g. to plasma (volume) chemistry. Terms like “antimicrobial reduction” indicate the purpose of the application, if it should be distinguished from others, e.g. “modification of wettability”.

The qualifier “plasma.source.specification” allows to define basic specifications of the plasma source, which are i) current/voltage waveform, ii) frequency range, iii) pressure range and iv) temperature range. These four specifications describe basic properties which can be applied to almost every plasma source and ensure a rough categorization of the plasma:

(i) “waveform” specifies the power delivery waveform and can take the values “pulsed”, “DC” (direct current), and “AC” (alternating current);
(ii) “frequency” specifies the pulse repetition frequency or the frequency of the waveform, and can take the values “low frequency” (< 300 kHz), “high frequency” (300 kHz to 300 MHz), and “microwave” (> 300 MHz). No value is to be added if “waveform” is set to “DC”;

(iii) “pressure” specifies the state of thermodynamic equilibrium and can take the values “low pressure” (∼ 10³ Pa), “medium pressure” (10³ to 10⁵ Pa), “atmospheric pressure” (≈ 10⁵ Pa), and “high pressure” (∼ 10⁶ Pa);

(iv) “temperature” specifies the gas temperature and can take the values “thermal” and “non-thermal”, which are fundamental categories to describe if a plasma is in local thermal equilibrium or not.

With the qualifier “plasma.source.properties” it is possible to add further description of plasma properties as free text. Finally, “plasma.source.procedure” is a free text container to describe procedures to set the plasma source into operation. But it can also be used to give details on the whole (experimental) setup needed to produce the data resource. Table 2 gives an overview over all qualifiers of the schema element “plasma.source”.

| Id | Field                      | Definition                                               | Format  | Example                                      |
|----|----------------------------|---------------------------------------------------------|---------|----------------------------------------------|
| 1.1| plasma.source.name         | name and/or type of the plasma source                   | term list | kINPen® MED, COST jet, HF plasma jet         |
| 1.2| plasma.source.application  | application the plasma source is applied for            | term list | plasma medicine, surface treatment, antimicrobial reduction |
| 1.3| plasma.source.specification| technical specifications of the plasma source (waveform, frequency, pressure, temperature) | controlled list | AC, high frequency, low pressure, non-thermal |
| 1.4| plasma.source.properties   | properties of the plasma source                          | free text | details on power input, current/voltage amplitude etc. |
| 1.5| plasma.source.procedure    | procedure to prepare the plasma source; this field should be used to described the whole procedure, including medium and target | free text | e.g. temperature conditioning for each parameter set |

The metadata collected by the schema element “plasma.source” are not mandatory and can be omitted if the dataset includes data which are not specific to a plasma source, e.g. data from target analysis. However, metadata for the plasma source should be included whenever applicable. For instance, the metadata of a plasma source used for pre-treatment of a specific target might also be included if the dataset contains only research data from target analysis.
2.2. Plasma medium

The schema element “plasma.medium” has three qualifiers and describes the medium the plasma is operated in or consisting of. First, “plasma.medium.name” names the medium. Examples are noble gases (e.g. Ar), molecular gases (e.g. CO$_2$), or complex mixtures, e.g. plasma compositions consisting of sulfur hexfluoride (SF$_6$) and polytetrafluoroethylene (PTFE). Arc plasmas operated in vacuum usually consist of evaporated electrode material like copper and chromium (Cu-Cr). For gas mixtures it is favourable to fill this field with a list of different species rather than to name each single mixture of species. Furthermore, chemical element symbols and common abbreviations are preferred, e.g. “Ar” instead of “argon” and “HMDSO” instead of “hexamethyldisiloxane”. Next, “plasma.medium.properties” is a free text qualifier that can take unstructured information to describe details of the plasma medium, e.g. gas flow rates, the carrier gas in a mixture, or the gas purity. Finally, “plasma.medium.procedure” is a free text container to describe procedures to prepare the medium before plasma operation and the treatment during plasma operation. Table 3 gives an overview over all qualifiers of the schema element “plasma.source”.

| Id | Field                     | Definition                                      | Format  | Example                                      |
|----|---------------------------|------------------------------------------------|---------|----------------------------------------------|
| 2.1| plasma.medium.name        | medium name the plasma source is operated in or acting on | term list | Ar, CO$_2$, H$_2$O, air                      |
| 2.2| plasma.medium.properties  | properties of the medium the plasma source is operated in or acting on | free text | gas flow rate: 100 sccm, carrier gas: Ar, precursor: HMDSO, gas mixture: Ar with 10 ppm HMDSO |
| 2.3| plasma.medium.procedure   | standard procedure to prepare the medium        | free text | gas flow has to be established for at least 30 s before plasma ignition. |

The schema element “plasma.medium” is not mandatory and can be omitted, e.g. if the description of the plasma source already provides sufficient information on the plasma medium. This might be the case, e.g. if the plasma source is a low-pressure sodium lamp, where the lamp fill is part of the plasma source specification. However, for reasons of findability redundant information on the plasma medium in the corresponding schema element is suggested.

2.3. Plasma target

As for “plasma.medium”, there are three qualifiers for the schema element “plasma.target” which allow to specify the name, properties, and procedure of the target. The qualifier “plasma.target.name” should designate the target the plasma source is acting on—either directly or mediated by a substance. Examples for possible target names are “Si wafer”, “distilled water” and “E. coli”. It is suggested to use chemical
element symbols or common abbreviations where applicable. Multiple targets can be named here. This is of particular importance if the action of the plasma is mediated by a substance. For instance, it may be of interest to treat water or pharmaceuticals in a plasma reactor and afterwards use those treated substances to let them interact with a cell line. Such cases are considered by specifying multiple plasma targets.

The qualifier “plasma.target.properties” is designed to collect details of the plasma target, e.g. geometric dimensions, grade, and orientation of a silicon wafer. Consequently, the qualifier “plasma.target.procedure” is eligible to describe any processing steps to prepare targets before plasma treatment (e.g. growth of cell lines) as well as handling throughout the plasma treatment.

| Id | Field                | Definition                                                                 | Format  | Example                                                                 |
|----|----------------------|---------------------------------------------------------------------------|---------|------------------------------------------------------------------------|
| 3.1| plasma.target.name  | name of the target the plasma source is acting on, either directly or mediated by a medium | term list | Si wafer, distilled water, Escherichia coli                           |
| 3.2| plasma.target.properties | properties of the target the plasma source is acting on              | free text | silicon wafer: 100 mm diameter, prime grade, orientation 100, E. coli (DSM 11250, NCTC 10538) |
| 3.3| plasma.target.procedure | standard procedure to prepare the target (pre-treatment) and handling throughout plasma treatment | free text | E. coli prepared on glass substrate according to internal procedure   |

The schema element “plasma.target” is not mandatory and can be omitted, e.g. if only the characterization of a plasma source is intended.

2.4. Diagnostics

The schema element “plasma.diagnostics” serves the purpose to give details on the respective plasma diagnostics and modelling/simulation procedures used to produce the data resource. This is of particular importance as in applied plasma physics numerous specialized diagnostic methods are relevant and filtering datasets according to the applied diagnostics can be helpful. Another advantage of this schema element is that datasets can be considered which are related to applied plasma physics but do not deal with a specific plasma source or plasma application. For instance, this is the case if a diagnostic or modelling/simulation method is reported which is not only applicable to plasmas but also to non-ionized gases, i.e. vapours or cold gas. Examples of plasma diagnostics names include “OES” (optical emission spectroscopy), “XPS” (X-ray photoelectron spectroscopy), “PIC-MCC” (particle-in-cell/Monte Carlo collision simulations). It is suggested to use common abbreviations where available.
The second qualifier “plasma.diagnostics.properties” contains further details on the applied diagnostics and modelling/simulation methods, respectively. References to journal publications with more details on the applied methods may be provided here. Table 5 gives an overview of all qualifiers of the schema element “plasma.diagnostics”.

| Id  | Field                  | Definition                                         | Format     | Example                             |
|-----|------------------------|----------------------------------------------------|------------|-------------------------------------|
| 4.1 | plasma.diagnostics.name | name of the applied diagnostics or modelling/simulation method | term list  | OES, LAAS, XPS, SEM, PIC-MCC, fluid-Poisson model |
| 4.2 | plasma.diagnostics.properties | details of the applied diagnostics which are not part of the resource metadata | free text  | laser diode at 395 nm and 50 mW |

The schema element “plasma.diagnostics” is mandatory because knowledge of the applied experimental/modelling/simulation method is assumed to be crucial for the reusability of the data.

2.5. Resource

The Plasma-MDS is designed to describe datasets which can contain several resources. Resources are digital representations of research data. Hence, the above defined metadata do not serve for the only purpose to describe a single resource but possibly a set of resources. To give details on the specifics of each resource, the schema element “plasma.resource” is introduced. The qualifiers might be in parts redundant to metadata of different metadata schemata like, e.g. Dublin Core and DataCite Metadata Schema. However, they provide key information on each resource which should be compiled into the schema element “plasma.resource” for the sake of clarity. The qualifiers are defined as follows:

(i) “filetype” obviously contains the file extension, e.g. pdf, csv or jpg;

(ii) “datatype” describes the type of data, which can take values like “data table”, “SEM image” (from scanning electron microscope), “cfu-plot” (colony forming units, e.g. of bacteria), to give some examples;

(iii) “range” is intended to detail a parameter range the resource is valid for. Examples might be a wavelength range (e.g. 400 to 800 nm in case of emission spectra), or a magnification and an accelerating voltage in case of scanning electron microscope images;

(iv) “quality” is considered to rank the level of scientific quality control. Allowed values are given by a controlled vocabulary consisting of “verified”, “published”, and “reviewed”. Here, “verified” is the lowest quality level and means that the resource is checked for plausibility by the data creators and the data curators. “published” means that the data of the resource have already been published in a peer-reviewed
paper. Finally, “reviewed” implies that the data resource has been peer-reviewed by an independent expert.

Table 6 provides an overview of all qualifiers of the schema element “plasma.resource”. This schema element is mandatory because information on the available resources is crucial for finding and selecting relevant datasets. Note that this element must be provided for each resource if several digital objects are attached to the dataset.

| Id | Field                  | Definition                                      | Format  | Example                              |
|----|-----------------------|-------------------------------------------------|---------|--------------------------------------|
| 5.1| plasma.resource.     | file type of the resource data                  | term list| csv, jpg, pdf                        |
|    | filetype              |                                                 |         |                                      |
| 5.2| plasma.resource.     | kind of digital data which are saved with the   | term list| data table, SEM image,               |
|    | datatype              | resource                                        |         | cfu-plot, high-speed video           |
| 5.3| plasma.resource.     | range in which the resource is valid            | free text| wavelength range:                    |
|    | range                 |                                                 |         | 400...800 nm                         |
| 5.4| plasma.resource.     | Data quality score                              | controlled| verified, published, reviewed        |
|    | quality               |                                                 | list    |                                      |

3. Examples

To demonstrate how Plasma-MDS can be used for the annotation of research data, two examples are provided in the following. The first example comes from basic research studies of order phenomena in atmospheric pressure plasma jets and does not involve a plasma target. The second example examines the origin of species in a liquid upon plasma interaction. Free access to the Plasma-MDS metadata of both examples is provided by INPTDAT—a new interdisciplinary data platform for plasma technology [18]. INPTDAT was built at INP with the aim to provide free and easy access to research data and information from all fields of applied plasma science and plasma medicine. It aims to support the findability, accessibility, interoperability and reuse of data for the low-temperature plasma community.

3.1. Correlation of helicality and rotation frequency of filaments in the ntAPPJ

The first example demonstrates how Plasma-MDS was used for the annotation of digital data that has been used for analysis of the correlation of helicality and rotation frequency of filaments in a non-thermal atmospheric pressure plasma jet (ntAPPJ) [19]. Parts of the dataset have been pictured in figure 4 in Schäfer et al. [20]. Tables 7 and 8 provide a preview of the Plasma-MDS metadata. Public access to the digital data and all metadata is provided by the dataset published with INPTDAT [21].
Table 7. Preview of Plasma-MDS metadata for the dataset “Correlation of helicality and rotation frequency of filaments in the ntAPPJ” [21]. Full access to all metadata is provided at [https://www.inptdat.de/node/43](https://www.inptdat.de/node/43).

| Id | Field              | Value                                                                                                                                                                                                 |
|----|--------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
|    | Plasma source      |                                                                                                                                                                                                        |
| 1.1| plasma.source.name | ntAPPJ, HF plasma jet                                                                                                                                                                                  |
| 1.2| plasma.source.application | PECVD                                                                                                                                                                                                   |
| 1.3| plasma.source.specification | AC, high frequency, atmospheric pressure, non-thermal                                                                                                                                               |
| 1.4| plasma.source.properties | Non-thermal atmospheric pressure plasma jet (capacitively coupled) operated in a self-organized regime (locked mode). Power: 7 to 9 W; Frequency: 27.12 MHz; Flow rate: 400 to 800 sccm argon; Electrodes: ring configuration, distance 5 mm, width 5 mm; Capillary: inner diameter 4 mm, outer diameter 6 mm |
| 1.5| plasma.source.procedure | The measurements occur 30 minutes after temperature conditioning of the plasma source for each parameter setting.                                                                                       |
|    | Plasma medium      |                                                                                                                                                                                                        |
| 2.1| plasma.medium.name | Ar                                                                                                                                                                                                     |
| 2.2| plasma.medium.properties | Flowrate: 0.4 to 0.8 slm; Pressure: 1 bar; Temperature: 300 to 1000 K; Purity: argon 6.0                                                                                                                                 |
| 2.3| plasma.medium.procedure | Standard conditions of the argon gas are assured.                                                                                                                                                      |
|    | Plasma target      |                                                                                                                                                                                                        |
| 3.1| plasma.target.name | –                                                                                                                                                                                                     |
| 3.2| plasma.target.properties | –                                                                                                                                                                                                     |
| 3.3| plasma.target.procedure | –                                                                                                                                                                                                     |
|    | Diagnostics        |                                                                                                                                                                                                        |
| 4.1| plasma.diagnostics.name | laser schlieren deflectometry, fast imaging                                                                                                                                                           |
| 4.2| plasma.diagnostics.properties | The filament behaviour has been visualized optically by means of imaging; The LSD set-up consists of a He-Ne laser (Linos) and a high-speed CMOS camera (Photon Focus). The displacement of the laser spot on the image sensor (pixel size: 8 µm, 1312 × 1082 pixels) of the camera is monitored ... |

3.2. Non-thermal plasma in contact with water: the origin of species

In the second example, Plasma-MDS was used for the annotation of a dataset published in the York Research Database [22]. This shows how Plasma-MDS and the research data platform INPTDAT can be used to improve the findability and reusability of digital research data published elsewhere. The dataset published with INPTDAT at [https://www.inptdat.de/node/98](https://www.inptdat.de/node/98) includes all Plasma-MDS metadata and refers to the original dataset published in the York Research Database [23]. In this case, detailed information on plasma source, plasma medium, plasma target, applied diagnostics, and published resources were extracted from the journal article and its supporting information [24] to which the digital data belong. Tables 9 and 10 provide a preview of the Plasma-MDS metadata. Here, INPTDAT does not provide direct access to the
Table 8. Preview of Plasma-MDS resource metadata for the dataset “Correlation of helicality and rotation frequency of filaments in the ntAPPJ” [21]. Full access to all resource metadata is provided at https://www.inptdat.de/node/84, https://www.inptdat.de/node/85, https://www.inptdat.de/node/86, https://www.inptdat.de/node/87.

| Id | Field                  | Resource 1       | Resource 2       | Resource 3       | Resource 4       |
|----|------------------------|------------------|------------------|------------------|------------------|
| 5.1| plasma.resource.filetype | png              | csv              | csv              | csv              |
| 5.2| plasma.resource.datatype | high-speed image | data table       | data table       | data table       |
| 5.3| plasma.resource.range   | Power: 7 to 9 W; Gas flow rate: 0.4 to 0.7 slm | Power: 7 W; Rotation frequency range: 0 to 90 Hz | Power: 8 W; Rotation frequency range: 0 to 90 Hz | Power: 9 W; Rotation frequency range: 0 to 90 Hz |
| 5.4| plasma.resource.quality | verified         | published        | published        | published        |

digital object, i.e. the research data but strongly enhances the findability and reusability of the original data by means of Plasma-MDS.

4. Discussion

The plasma metadata schema Plasma-MDS was developed to complement basic metadata schemata with metadata fields for the collection of domain-specific information. This was demonstrated by means of two examples (cf. tables 7–10). This section discusses how Plasma-MDS supports the transfer of FAIR data principles (cf. table 1) into practice to enable data driven plasma science.

4.1. Findability

To be findable, machine readable metadata should allow the discovery of relevant datasets by humans and computer systems [25]. According to requirement F1 in table 1 a globally unique and persistent identifier should be assigned to each dataset. This identifier allows to find, track and cite data and their metadata. Plasma-MDS is not needed to meet this requirement because metadata fields for the unique identifier are already part of basic metadata schemata (e.g. Dublin Core metadata field “identifier”). However, Plasma-MDS strongly supports the fulfilment of requirement F2 in table 1 by providing specific fields to collect rich domain-specific metadata. The metadata collected by Plasma-MDS aims to allow researchers to properly understand the nature of the dataset by including descriptive information about the context, conditions, and quality of the data as demonstrated by the two examples in tables 7–10. Particularly, the metadata fields using controlled lists (plasma.source.specification and plasma.resource.quality) and term lists (e.g. qualifier “name” for all schema elements) also support the automated processing of metadata by computer systems. The collection
Table 9. Preview of Plasma-MDS metadata for the dataset “Non-thermal plasma in contact with water: the origin of species” [23]. Full access to all metadata is provided at [https://www.inptdat.de/node/98](https://www.inptdat.de/node/98).

| Id | Field                                      | Value                                                                                                                                 |
|----|--------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------|
|    | Plasma source                              |                                                                                                                                             |
| 1.1| plasma.source.name                         | kHz plasma jet, CAP                                                                                                                          |
| 1.2| plasma.source.application                  | reactive species generation                                                                                                                   |
| 1.3| plasma.source.specification                | AC, low frequency, atmospheric pressure, non-thermal                                                                                          |
| 1.4| plasma.source.properties                   | The plasma was ignited in a quartz tube (4 mm ID and 6 mm OD, 100 mm length) surrounded by copper electrodes (10 mm width) separated by 20 mm. A PVM500 Plasma... |
| 1.5| plasma.source.procedure                    | In a typical experiment, 100 µL of liquid sample was placed in a well on top of a glass stand inside the reactor. The distance from the nozzle to the sample was 10 mm unless... |
|    | Plasma medium                              |                                                                                                                                             |
| 2.1| plasma.medium.name                         | He, H$_2$O                                                                                                                                  |
| 2.2| plasma.medium.properties                   | The plasma was operated with a feed gas of helium with oxygen and water admixtures controlled by mass flow controllers (MFCs) (Brooks Instruments and Brooks... |
| 2.3| plasma.medium.procedure                    | The experiments involving different feed gas humidity were performed by using split helium flow (i.e., by mixing dry helium with water-saturated helium in desired proportions)... |
|    | Plasma target                              |                                                                                                                                             |
| 3.1| plasma.target.name                         | H$_2$O$_2$, H$_2$SO$_4$, NaN$_3$, D$_2$O, PBN, TEMP, TEMPO, sodium tosylate, H$_2$O, DMPO, DEPMPO, potassium bis(oxalato)oxotitanate(IV) dihydrate |
| 3.2| plasma.target.properties                   | Hydrogen peroxide H$_2$O$_2$ (30%), sulphuric acid H$_2$SO$_4$ (>95%) and sodium azide NaN$_3$ (≥99.5%) were purchased from Fluka. Deuterium oxide D$_2$O (99.9 atom % D),... |
| 3.3| plasma.target.procedure                    | In spin trapping experiments, a 100 mM solution of a spin trap (PBN, DMPO or DEPMPO) was prepared in H$_2$O, H$_2$O$_2$ or D$_2$O. Ozone was measured in 60 mM aqueous... |
|    | Diagnostics                                |                                                                                                                                             |
| 4.1| plasma.diagnostics.name                    | spin-trapping, isotopic labelling, EPR spectroscopy, OES                                                                                     |
| 4.2| plasma.diagnostics.properties              | A high voltage probe (Tektronix P6015A) and current probe (Ion Physics Corporation CM-100-L) were used with a Teledyne LeCroy WaveJet 354A oscilloscope to measure time... |

of general information (e.g. creator, date, and license) is already supported by basic metadata schemata (Dublin Core, DataCite Metadata Schema, and others). These basic metadata schemata also meet the requirement F3 in table [1] by providing metadata fields...
Table 10. Preview of Plasma-MDS resource metadata for the dataset “Non-thermal plasma in contact with water: the origin of species” [23]. Full access to all resource metadata is provided at [https://www.inptdat.de/node/99](https://www.inptdat.de/node/99).

| Id  | Field                     | Value                                                                 |
|-----|---------------------------|----------------------------------------------------------------------|
| 5.1 | plasma.resource.filetype  | html                                                                 |
| 5.2 | plasma.resource.datatype  | external resource                                                     |
| 5.3 | plasma.resource.range     | The results of the plasma exposure of the samples (e.g., the absolute values of concentration of DMPO-OH) were largely affected by small changes in the configuration of the jet, such as the electrodes contact with the quartz tube, the depth of the tube protrusion inside the reactor, and the vertical alignment of the tube. However, while the numerical values changed, the observed trends remained persistent. For example, the concentration of DMPO-OH increased with the initial introduction of H$_2$O to He feed gas and decreased with higher H$_2$O content, the concentration of DMPO-OH was lower at 4 mm distance than 10 mm, etc. Thus, the error assessment was performed within a set configuration of the jet for several conditions. Conditions of less uniform plasma nature (i.e., in the presence of large amounts of admixtures in the feed gas) generally lead to an increase in standard deviation of the concentration values. The maximum deviation from the mean was found to be ca. 12%. |
| 5.4 | plasma.resource.quality   | published                                                             |

to register license information (e.g. Dublin Core metadata field “rights”).

To take full advantage of the benefits of Plasma-MDS and fulfil the requirement F4 in table 1 (indexing of metadata in a searchable resource), the implementation of Plasma-MDS in a (meta)data repository is needed. However, generic or institutional data repositories usually do not provide the possibility to collect domain-specific information on deposited datasets. INPTDAT ([https://www.inptdat.de](https://www.inptdat.de)) is the first data platform that implements Plasma-MDS and indexes the domain-specific metadata to provide elaborate search features for interdisciplinary datasets in the field of plasma technology.

4.2. Accessibility

To be accessible, data and metadata should be stored for the long term such that they can be easily accessed by humans and computer systems using standard communication protocols. This requirement cannot be met by the metadata schema itself, but by the repository in which the (meta)data is stored. Any (meta)data repository providing Plasma-MDS as metadata schema should meet the requirements for accessibility A1, A1.1, A1.2, and A2 in table 1. Therefore, the data platform INPTDAT uses public APIs (application programming interfaces) to provide open access to general as well as
domain-specific metadata in JSON-LD format (requirements A1 and A1.1 in table 1). No authentication and authorization of users is required to access metadata (requirement A1.2 in table 1). To meet the requirement A2 (long-term accessibility of metadata), INPTDAT maintains all metadata physically separated from data files and provides the possibility to easily extract and move metadata to other repositories by public APIs.

4.3. Interoperability

To be interoperable, data should be ready to be exchanged, interpreted, and combined in a (semi)automated way with other datasets by humans and computer systems [25]. Therefore, community standards for data management and, in particular, established vocabularies/ontologies/thesauri are required (cf. requirement I1 in table 1). In this respect, Plasma-MDS can be seen as a first step towards increasing awareness and the development of a common standard. In order to be able to meet requirement I2 in table 1 in the future, appropriate collaborative structures are to be set up that allow to develop, maintain, and document controlled vocabularies that themselves again fulfil the FAIR principles. Finally, the possibility to include qualified references to other (meta)data (cf. requirement I3 in table 1) is provided by basic metadata schemata (e.g. Dublin Core metadata field “relation”).

4.4. Reusability

To be reusable, the provided metadata must ensure that the dataset can be used in future research and that it can be integrated with other compatible data sources. The conditions under which the data can be reused should be clear to humans as well as computer systems [25]. Therefore, requirement R1 in table 1 demands a detailed description of the dataset including information on what the dataset contains, how it was generated and processed, and the conditions under which the data can be reused. Future use of Plasma-MDS will turn out whether the implemented qualifiers for the schema elements “plasma.source”, “plasma.medium”, “plasma.target”, “plasma.diagnostics”, and “plasma.resource” suffice to achieve this requirement and which adaptions might be necessary in revised versions of Plasma-MDS. It is worth mentioning that each metadata schema is not fixed but subject to regular updates. Furthermore, it is important to note that metadata schemata are only as good as they are being used. It is the responsibility of users to provide the required information with their data.

The requirement R1.1 in table 1 can be met without using Plasma-MDS. Basic metadata schemata provide fields to include information on the data usage license (e.g. Dublin Core metadata field “rights”). A discussion of appropriate licenses for data publications is beyond the scope of this paper. In general, the Creative Commons (CC) license CC BY 4.0 [26] is recommendable for research data publications. More information and recommendations on how to license research data are given in Ref. [27].

Requirement R1.2 in table 1, namely the association of data with detailed provenance, appears to be the most challenging FAIR data principle. At the same
time, it is the most important precondition for reliable reuse of research data. Detailed information about the provenance of data allows researchers to understand how the data were generated, in which context it can be reused, and how reliable it is. With the qualifiers “properties” and “procedure” for the different schema elements, Plasma-MDS is prepared to collect the relevant metadata. However, it is difficult to ensure that third parties will be able to fully understand and reproduce the workflow of data creation, especially for the large number of experiments in the field of low-temperature plasmas for which no standard operation procedures (SOPs) are available yet. In this respect, Plasma-MDS may give the impetus to agree on certain SOPs and data annotation standards for widely used experiments in the low-temperature plasma community. This would also support the fulfilment of requirement R1.3 in table 1 demanding that data and metadata meet domain-relevant community standards. Obviously, this requirement is only applicable if community standards or best practices for data archiving and sharing exist. Plasma-MDS can possibly contribute to the establishment of such standards.

5. Summary and outlook

With Plasma-MDS, the first metadata schema was introduced for the documentation of research data in the field of applied plasma science and plasma medicine. In accordance with typical plasma processes and applications, the schema contains metadata fields to collect annotations about the plasma source, plasma medium, and plasma target involved in the study from which research data were obtained. Furthermore, metadata for the respectively applied diagnostic and modelling/simulation methods are collected. Finally, resource metadata fields are included to describe the individual digital objects belonging to the dataset. It was discussed how these schema elements support research data management in accordance with the FAIR data principles. The discussion revealed that the use of Plasma-MDS as a supplement to basic metadata schemata, that are available for collection of general (domain-independent) information, strongly improves the possibilities for “fair” research data management in the area of plasma technology.

However, there is still a need for action, particularly in the establishment of community standards. In this regard there is the desire that Plasma-MDS will be integrated into other data repositories and further developed by the plasma community. The establishment of research data management standards in widespread plasma research areas is seen as a basic prerequisite for extensive data-driven research and will be followed up in the initiative on data-driven plasma science [13, 28]. The long-term goal is to establish Plasma-MDS as a widespread community standard, which supports the reuse of research data and promotes data-driven plasma science up to the point where research data management becomes everyday practice in the plasma community.
Acknowledgement

The work was funded by the Federal Ministry of Education and Research (BMBF) under the grant marks 16FDM005 and 16QK03A. MMB thanks D. Loffhagen and D. Uhrlandt for supportive discussions and the scientists involved at INP for helpful suggestions for the design of the metadata schema. The responsibility for the content of this publication lies with the authors.

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