|  |  |  |
| --- | --- | --- |
| **Report IDM reference No.** | EFDA\_D\_2MVQWL | **Version: see IDM** |

Final Report

on Deliverable

MAT-1.2.2-T011-D001 - Database Population - Functional Materials for year 2016

|  |  |  |  |
| --- | --- | --- | --- |
|  | | **Deliverable-ID**[[1]](#footnote-1) | MAT-1.2.2-T011-D001 |
| **Work Package** | *WPMAT* | **Date** | *31st Oct. 2016* |
| **Project Leader** | *Michael Rieth* | | |
|  | | | |
| **TS Title** | Summary overview report on Database Population- Functional Materials for year 2016 | | |
| **TS Ref. No.** | MAT-1.2.2-T011 | **TS IDM-link** | *EFDA\_D\_2MRK2N* |
| **Task Owner** | *Ferenc Gillemot* | | |
| **RU(s)** | *MTA EK* | | |

|  |  |
| --- | --- |
| **Report Review & Approval** | |
| **IDM role** | **Name(s)** |
| **Author** | Ferenc Gillemot |
| **Co-author(s)** | *Ildiko Szenthe, Attila Kovács* |
| **Reviewer(s)** | *Michael Gorley* |
| **PMU Reviewer** | *Eberhard Diegele, Matti Oron-Carl* |
| **Approver** | *Michael Rieth* |

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| x | Study / Assessment |  | Procurement / Commissioning of Hardware |  | Industry |

|  |  |  |  |
| --- | --- | --- | --- |
|  | Use of Facility |  | Other *{please specify}* |

|  |
| --- |
| **Executive Summary** |
| The purpose of the work is to create and populate material database infrastructure for the materials of the DEMO in vessel components, for functional materials. Functional materials are different from the structural materials. The strengths properties have secondary importance for the designers, but some physical properties such as electrical resistivity, electrical conductivity, permittivity, dielectric strengths, loss of tangent (dissipation factor), transmission, absorption and reflectance are the more relevant properties. The objective of the work to start to collect these properties and prepare data sources for the first draft of functional materials MPH. MTA EK fulfilled the tasks, collected large amount of data. All reports on IDM have been evaluated, the data uploaded into the database. |

|  |
| --- |
| **Comments** (shortcomings, deviations, etc.) |
| The co-operation between the Functional Materials Group and the database should be enhanced. We recommend in 2017 to organise a VC with all Functional Material Group participants on data supply and MPH in every quarter of the year, and a special day together with the FM monitoring at June, or separately. |

**Table of Contents**

[1 Short Introduction and Objectives of Work 3](#_Toc401047476)

[2 Description of Work 4](#_Toc401047477)

[3 Conclusion 4](#_Toc401047478)

[4 References 5](#_Toc401047479)

**Abbreviations**

|  |  |
| --- | --- |
| *FM* | *Functional Materials* |
| *DEMO* | *Demonstration Fusion Reactor* |
| *MPH* | *Material Properties Handbook* |
| *MTA EK* | *Energy Reserach Centre of the Hungarian Academy of Sciences* |
| VC | Video Conference |

# Short Introduction and Objectives of Work

In 2014 the database structure has been developed for (armour, structure, functional, joint) including developing the data collection templates and the format of these templates should be consistent across the differing materials where possible. To prepare a good database containing one type of materials is a difficult task. It should be user friendly, can include all relevant information, etc. The development has several steps: study the relevant standards and codes, elaborate a structure, test it on virtual and existing real data etc. If the database have to be harmonized for very different materials ,then the task is even more difficult. MTA EK developed a harmonized database for armour, structure, functional materials and joints. Only two contributions suggesting very slight modifications arrived (to include two more fields). In 2015 decision were made, that only the functional materials database have to be managed by MTA EK, and the existing database on the other materials will be used. The decision is understandable since data conversion from one database to an another is not easy, and increases the probability of typing errors. On the other hand, if this decision was made earlier it should save a lot of wasted efforts, and compromises used at the development of functional materials database. Further difficulty was, that MTA EK had experience in the field of development and use of databases, but the properties of the functional materials were outside of their practice, it slows down the work. Due to this situation in 2015 the database structure had to be upgraded and simplified, tested with the available data and sent to the functional materials group for comments. No comments again. MTA EK participated on the FM monitoring meetings, introduced the database, asked the research owners to provide data.

The objective of the 2016 year was focus on data collection and interaction with relevant WPMAT sub-projects in support of the EDDI database and MPH developments.

# Description of Work

Several subtask included into the work.

a. Engagement with WPMAT sub-project team in Functional Materials (FM), including attendance at their PMM and additional key meetings; in agreement with EDDI project leader, keep the FM group updated on EDDI developments, including: evolution of database templates, Materials Property Handbook, Demo Design Criteria, Materials Management Framework and Testing (presenting where necessary). MTA EK participated on the June PMM meeting at Tartu and presented the database and FM MPH, required contribution of the participants. At middle of August 2016 the database, the templates and the draft MPH have been sent to the FM participants asking for data and assistance in the development from them.

b. Template Development: Work with the FM group (and other EDDI groups including KIT) to continue development and consistent formatting of data collection templates. The development of the templates made in two directions: partly at upload of literature and report data the missing fields have been replaced (three cases), partially the templates have been introduced on the FM meeting and sent to the participants for corrections and extensions.

c. Data collection. All existing FM report downloaded, read, and the available data collected and uploaded into the database. Parallel with this work literature data also had been collected and uploaded. Every data was discussed, and evaluated. Decision was made whether the data can be included into the database as number, or in other format: diagram in the case of too many data points, or picture (e.g. microscopy picture on grain size). Data from reports are more preferable (the progress report author is responsible for the report content), the open publications are not responsible for the data. At open publications the excellence of the publishing institution and the comparison with other data is the degree of the data acceptance. Most data published in diagram format, and have been re-digitalised. It is a time consuming work, and decreases the reliability of the data. In future the direct supply of numeric data has to be organised.

d. Data Integrity for Qualification: The collated functional materials data have been reviewed against EUROFUSION EDDI database quality thresholds ([2M9HTV](https://idm.euro-fusion.org/IDM/Pages/DocumentView.aspx?uid=2M9HTV)) and selected data have been upload into the database. (EFDA\_D\_2MRLZK v1.0)

e. Data collection: more than 140 new records collected, evaluated and uploaded into the database. All reports uploaded into the IDM have been read, evaluated and relevant data uploaded into the database. Unfortunately many reports haven't identified properly the tested materials, or they are presented only on conferences. Hopefully these data will be sent until the end of November to the MTA EK to include into the database.

# Conclusion

Large number of data collected, uploaded and used for the Functional Material MPH. MTA EK participated on the Functional Materials monitoring meetings. The co-operation between the Functional Materials Group and the database should be enhanced. We recommend in 2017 to organise a VC with all Functional Material Group participants on data supply and MPH in every quarter of the year, and a special day together with the FM monitoring at June, or separately. MTA EK welcomes the FM group meeting at 2017.

The objective of the work was to collect the functional material properties and prepare data sources for the first draft of functional materials MPH. MTA EK fulfilled the tasks, collected large amount of data and these data used to elaborate the pilot MPH on alumina. All reports on IDM have been evaluated, the data uploaded into the database.

# References

1. O. Sidletskiy et al.: „Structure property correlations in a Ce doped Lu, Gd, 2SiO5 Ce scintillator”. Cryst. Growth Des. 12 2012 4411 4416
2. Lushchik et al.: “Influence of complex impurity centres on radiation damage in wide-gap metal oxides”. Nuclear Instruments and Methods in Physics Research Section B Beam Interactions with Materials and Atoms August 2015
3. R. Zabels et al.: “Depth profiles of indentation hardness and dislocation mobility in MgO single crystals irradiated with swift 84Kr and 14N ions” Appl. Phys
4. J. Mollii, et all: “Insulator dielectric properties during irradiation and influence of RIED effect” Journal of Nuclear Materials 212-215 (1994) 1113-1118
5. Uberuaga P B et al.: „Opposite correlations between cation disordering and amorphization resistance in spinels versus pyrochlores“ Nature Communications 29 October 2015
6. Gilbert C A et al. „A theoretical study of intrinsic point defects and defect clusters in magnesium aluminate spinel“ J. Phys. Condens. Matter 21 (2009)
7. Sawai S and Uchino T: „Visible photoluminescence from MgAl2O4 spinel with cation disorder and oxygen vacancy“, J. Appl. Phys. 112 (2012) 103523
8. Ibarra et al.: “High dose neutron irradiation of MgAl2O4 spinel effects of post irradiation thermal annealing on EPR and optical absorption” Journal of Nuclear Materials 336 (2005) 156–162
9. Gritsyna V T et al.: „Optical transitions in magnesium aluminate spinel crystals of different composition exposed to irradiation” Nucl. Instr. and Meth. B 218 (2004) 264–270
10. Yu. F. Zhukovskii, et al.: “Ab initio simulations on migration paths of interstitial oxygen in corundum”, Nucl. Instr. Meth. B, in press
11. Mota et al: “Calculation of damage function of Al2O3 in irradiation facilities for fusion reactor applications”. J. Nucl. Mater. 442, S699-S704 (2013)
12. A. Serikov et al:“Neutronics analysis for ITER cable looms” Fusion Engineering and Design 96–97 (2015) 943–947
13. T. Brudevoll, et all: “Interstitial oxygen atom diffusion in MgO”. Phys. Rev. B 53, 7731–7735 (1996).
14. E.A. Kotomin et al: “Kinetics of *F* Center Annealing and Colloid Formation in Al2O3” J. Nucl. Mater. 442 \*2013( 5699)
15. B. Evans: “A review of the optical properties of anion lattice vacancies, and electrical conduction in -A1203: their relation to radiation-induced electrical degradation” Journal of Nuclear Materials 219 (1995) 202-223
16. Danilov, R. Heidinger, “New approach for open resonator analysis for dielectric measurement at mm-wavelength” Journal of the European Ceramic Society 23 (2003) 2623–2626
17. R. Vila at al: “Thermally Stimulated Depolarization Currents In Neutron Irradiated Al203” Solid State Communications, Vol. 79, No. 4, Pp. 295-297, 1991
18. R. Vila, et all: “Dielectric spectroscopy of alumina ceramics over a wide frequency range”, J. Nucl. Mater. 253 (1998) 141–148

1. One *Deliverable Report* shall be submitted for each deliverable e.g. Study Report, Commissioning Report, Final Assessment Report, Technical Acceptance Report, Procurement Report, etc. [↑](#footnote-ref-1)