



NIST/RDA DTR Demonstration Application:

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research data sharing without barriers

rd-alliance.org

■ Participants

NIST MML & ITL Labs

WGs DTR & PID: CNRI & DKRZ

Dakota Consulting & Kent State University

■ Motivation:

– Common problem:

What kind of data have I found? What can I do with it?

– Materials Science & Engineering focus:

Find plottable XRD data via NIST Mat'ls Resource Registry

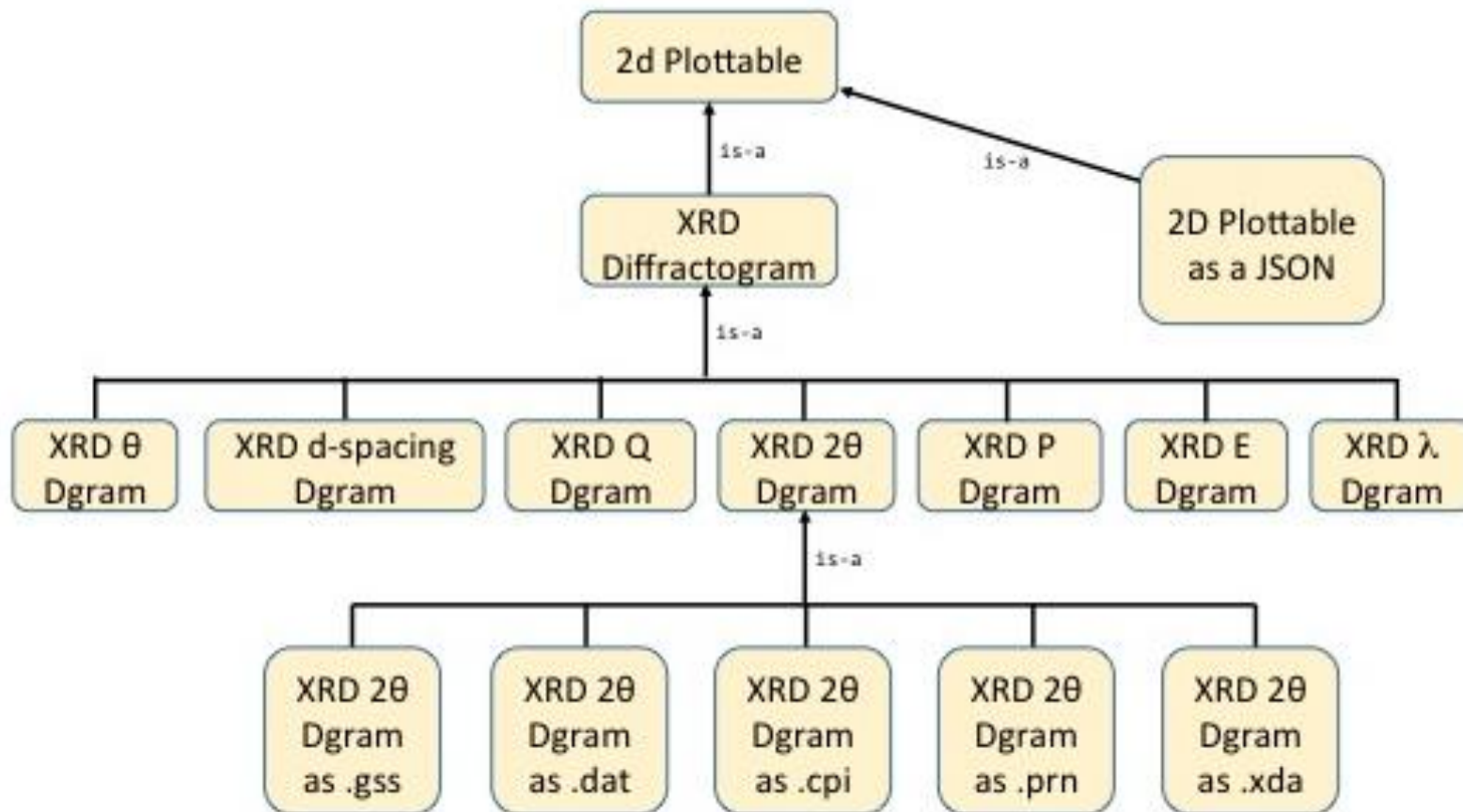
Data Curator System, & Data Repository

Can Data Type Registry help?

- name
- description
- provenance
 - contributors
 - creation date
 - last mod date
- Expected Uses
- Representation and Semantics
 - expression :: value :: details
- Properties (build on other types)
 - name
 - TID of existing type
 - representation and semantics
- Relationship
 - name :: relative names :: details

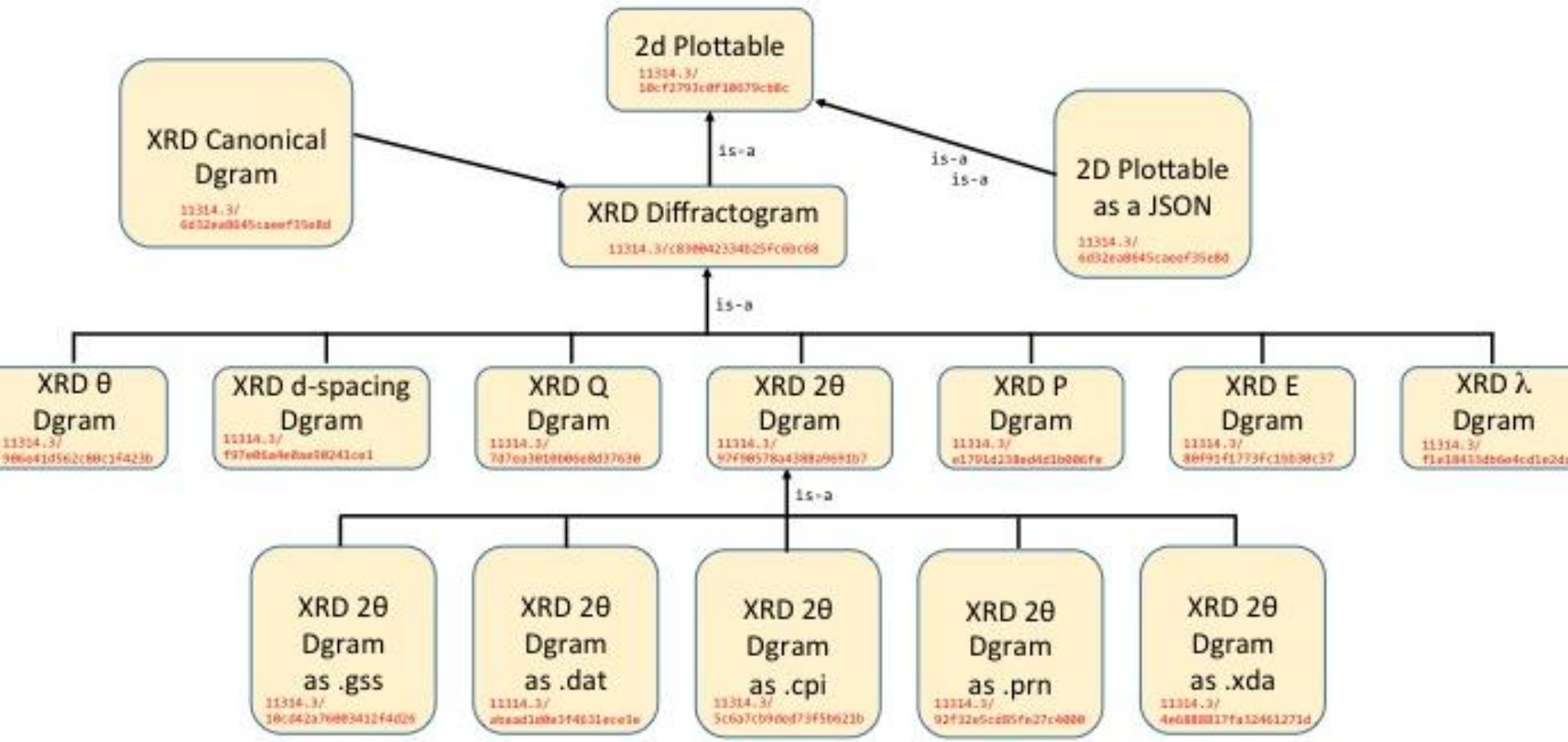
Slide prepared by John Henry Scott, MML, NIST

RDA Demo XRD Data Types



Slide prepared by John Henry Scott, MML, NIST

RDA Demo XRD Data Types



2D Plottable

```
{
  "identifier" : "11314.3/10cf2793c0f10679cb8c",
  "name" : "RDA-Demo 2D Plottable",
  "description" : "Data in a form suitable for plotting as a 2D line profile with X and Y axes",
  "provenance" : {
    "contributors" : [ {
      "identifiedUsing" : "ORCID",
      "name" : "0000-0002-3796-2110",
      "details" : "John Henry J. Scott, http://orcid.org/0000-0002-3796-2110"
    } ],
    "creationDate" : "2015-07-01T14:20:58.084Z",
    "lastModificationDate" : "2015-07-01T15:23:42.052Z"
  },
  "expectedUses" : [ "RDA/MGI DTR Demonstration" ],
  "relationships" : [ {
    "name" : "has-subtype",
    "relativeNames" : [ "11314.3/c830042334b25fc6bc68", "11314.3/906e41d562c80c1f423b",
"11314.3/f97e06a4e0ae90241ce1", "11314.3/7d7ea3010b06e8d37630", "11314.3/97f90578a4388a9691b7",
"11314.3/e1791d238ed4d1b006fe", "11314.3/80f91f1773fc1bb30c37", "11314.3/f1e18433db6e4cd1e2da",
"11314.3/10cd42a76003412f4d26", "11314.3/abaad1d0e3f4631ece3e", "11314.3/5c6a7cb9ded73f5b621b",
"11314.3/92f32e5cd85fe27c4000", "11314.3/4e6888817fa32461271d" ]
  }, {
    "name" : "has-child",
    "relativeNames" : [ "11314.3/c830042334b25fc6bc68" ]
  } ]
}
```

2D Plottable as JSON

```
{
  "identifier" : "11314.3/6d32ea8645caeef35e8d",
  "name" : "RDA-Demo 2D Plottable as JSON",
  "description" : "Data in a form suitable for plotting as a 2D line profile with X and Y axes,
serialized in a specific JSON representation",
  "provenance" : {
    "contributors" : [ {
      "identifiedUsing" : "ORCID",
      "name" : "0000-0002-3796-2110",
      "details" : "John Henry J. Scott, http://orcid.org/0000-0002-3796-2110"
    } ],
    "creationDate" : "2015-07-01T19:14:24.724Z",
    "lastModificationDate" : "2015-07-01T19:14:26.362Z"
  },
  "expectedUses" : [ "RDA/MGI DTR Demonstration" ],
  "relationships" : [ {
    "name" : "is-a",
    "relativeNames" : [ "11314.3/10cf2793c0f10679cb8c" ]
  }, {
    "name" : "has-parent",
    "relativeNames" : [ "11314.3/10cf2793c0f10679cb8c" ]
  } ]
}
```

XRD Diffractogram

```
{
  "identifier" : "11314.3/c830042334b25fc6bc68",
  "name" : "RDA-Demo XRD Diffractogram",
  "description" : "A generic X-ray Diffraction (XRD) Diffractogram containing data on the angular scattering distribution of X-rays from a sample, expressed in any of a large number of different variations.",
  "provenance" : {
    "contributors" : [ {
      "identifiedUsing" : "ORCID",
      "name" : "0000-0002-3796-2110",
      "details" : "John Henry J. Scott, http://orcid.org/0000-0002-3796-2110"
    } ],
    "creationDate" : "2015-07-01T14:30:20.302Z",
    "lastModificationDate" : "2015-07-01T18:39:11.259Z"
  },
  "expectedUses" : [ "RDA/MGI DTR Demonstration" ],
  "relationships" : [ {
    "name" : "is-a",
    "relativeNames" : [ "11314.3/10cf2793c0f10679cb8c" ]
  }, {
    "name" : "has-subtype",
    "relativeNames" : [ "11314.3/906e41d562c80c1f423b", "11314.3/f97e06a4e0ae90241ce1",
"11314.3/7d7ea3010b06e8d37630", "11314.3/97f90578a4388a9691b7", "11314.3/e1791d238ed4d1b006fe",
"11314.3/80f91f1773fc1bb30c37", "11314.3/f1e18433db6e4cd1e2da", "11314.3/10cd42a76003412f4d26",
"11314.3/abaad1d0e3f4631ece3e", "11314.3/5c6a7cb9ded73f5b621b", "11314.3/92f32e5cd85fe27c4000",
"11314.3/4e6888817fa32461271d" ]
  }, {
    "name" : "has-child",
    "relativeNames" : [ "11314.3/906e41d562c80c1f423b", "11314.3/f97e06a4e0ae90241ce1",
"11314.3/7d7ea3010b06e8d37630", "11314.3/97f90578a4388a9691b7", "11314.3/e1791d238ed4d1b006fe",
"11314.3/80f91f1773fc1bb30c37", "11314.3/f1e18433db6e4cd1e2da" ]
  }, {
    "name" : "has-parent",
    "relativeNames" : [ "11314.3/10cf2793c0f10679cb8c" ]
  } ]
} ]
```


XRD Canonical Diffractogram

```
{
  "identifier" : "11314.3/e3b14757012a675a6ea1",
  "name" : "RDA-Demo XRD Canonical Diffractogram",
  "description" : "A generic X-ray Diffraction (XRD) Canonical Diffractogram containing data on the angular scattering distribution of X-rays from a sample, expressed as scattered X-ray intensity versus twice the scattering angle (2-Theta, measured in units of degrees), and serialized in any of a large number of different formats. This format is supported by the NIST Material Data Curation System (MDCS).",
  "provenance" : {
    "contributors" : [ {
      "identifiedUsing" : "ORCID",
      "name" : "0000-0002-3796-2110",
      "details" : "John Henry J. Scott, http://orcid.org/0000-0002-3796-2110"
    }, {
      "identifiedUsing" : "ORCID",
      "name" : "0000-0002-3026-4408",
      "details" : "Antoine Fillinger, http://orcid.org/0000-0002-3026-4408"
    } ],
    "creationDate" : "2015-09-08T19:38:06.235Z",
    "lastModificationDate" : "2015-09-08T19:38:06.323Z"
  },
  "expectedUses" : [ "RDA/MGI DTR Demonstration" ],
  "relationships" : [ {
    "name" : "is-a",
    "relativeNames" : [ "11314.3/10cf2793c0f10679cb8c", "11314.3/c830042334b25fc6bc68" ]
  }, {
    "name" : "has-parent",
    "relativeNames" : [ "11314.3/c830042334b25fc6bc68" ]
  } ]
}
```

XRD 2-Theta Diffractogram

```
{
  "identifier" : "11314.3/97f90578a4388a9691b7",
  "name" : "RDA-Demo XRD 2-Theta Diffractogram",
  "description" : "A generic X-ray Diffraction (XRD) Diffractogram containing data on the angular scattering distribution of X-rays from a sample, expressed as scattered X-ray intensity versus twice the scattering angle (2-Theta, measured in units of degrees), and serialized in any of a large number of different formats.",
  "provenance" : {
    "contributors" : [ {
      "identifiedUsing" : "ORCID",
      "name" : "0000-0002-3796-2110",
      "details" : "John Henry J. Scott, http://orcid.org/0000-0002-3796-2110"
    } ],
    "creationDate" : "2015-07-01T14:43:13.375Z",
    "lastModificationDate" : "2015-07-01T18:37:27.313Z"
  },
  "expectedUses" : [ "RDA/MGI DTR Demonstration" ],
  "relationships" : [ {
    "name" : "is-a",
    "relativeNames" : [ "11314.3/10cf2793c0f10679cb8c", "11314.3/c830042334b25fc6bc68" ]
  }, {
    "name" : "has-subtype",
    "relativeNames" : [ "11314.3/10cd42a76003412f4d26", "11314.3/abaad1d0e3f4631ece3e", "11314.3/5c6a7cb9ded73f5b621b", "11314.3/92f32e5cd85fe27c4000", "11314.3/4e6888817fa32461271d" ]
  }, {
    "name" : "has-child",
    "relativeNames" : [ "11314.3/10cd42a76003412f4d26", "11314.3/abaad1d0e3f4631ece3e", "11314.3/5c6a7cb9ded73f5b621b", "11314.3/92f32e5cd85fe27c4000", "11314.3/4e6888817fa32461271d" ]
  }, {
    "name" : "has-parent",
    "relativeNames" : [ "11314.3/c830042334b25fc6bc68" ]
  } ]
}
```

XRD 2-Theta Diffractogram as GSAS

```
{
  "identifier" : "11314.3/10cd42a76003412f4d26",
  "name" : "RDA-Demo XRD 2-Theta Diffractogram as GSAS",
  "description" : "An X-ray Diffraction (XRD) Diffractogram containing data on the angular
scattering distribution of X-rays from a sample, expressed as scattered X-ray intensity versus
twice the scattering angle (2-Theta, measured in units of degrees), and serialized in the GSAS
format.",
  "provenance" : {
    "contributors" : [ {
      "identifiedUsing" : "ORCID",
      "name" : "0000-0002-3796-2110",
      "details" : "John Henry J. Scott, http://orcid.org/0000-0002-3796-2110"
    } ],
    "creationDate" : "2015-07-01T15:03:05.158Z",
    "lastModificationDate" : "2015-07-01T18:41:58.324Z"
  },
  "expectedUses" : [ "RDA/MGI DTR Demonstration" ],
  "relationships" : [ {
    "name" : "is-a",
    "relativeNames" : [ "11314.3/10cf2793c0f10679cb8c", "11314.3/c830042334b25fc6bc68",
"11314.3/97f90578a4388a9691b7" ]
  }, {
    "name" : "has-parent",
    "relativeNames" : [ "11314.3/97f90578a4388a9691b7" ]
  } ]
}
```

XRD 2-Theta Diffractogram as .dat

```
{
  "identifier" : "11314.3/abaad1d0e3f4631ece3e",
  "name" : "RDA-Demo XRD 2-Theta Diffractogram as .dat",
  "description" : "An X-ray Diffraction (XRD) Diffractogram containing data on the angular
scattering distribution of X-rays from a sample, expressed as scattered X-ray intensity versus
twice the scattering angle (2-Theta, measured in units of degrees), and serialized in the .dat
format.",
  "provenance" : {
    "contributors" : [ {
      "identifiedUsing" : "ORCID",
      "name" : "0000-0002-3796-2110",
      "details" : "John Henry J. Scott, http://orcid.org/0000-0002-3796-2110"
    } ],
    "creationDate" : "2015-07-01T15:04:58.295Z",
    "lastModificationDate" : "2015-07-01T18:42:53.412Z"
  },
  "expectedUses" : [ "RDA/MGI DTR Demonstration" ],
  "relationships" : [ {
    "name" : "is-a",
    "relativeNames" : [ "11314.3/10cf2793c0f10679cb8c", "11314.3/c830042334b25fc6bc68",
"11314.3/97f90578a4388a9691b7" ]
  }, {
    "name" : "has-parent",
    "relativeNames" : [ "11314.3/97f90578a4388a9691b7" ]
  } ]
}
```

Experimentation Showcase: 10:30-11:00 Textiles Room

- A user looks for x-ray diffraction data on Aluminum Oxide (Al^2O^3) & limits the search to diffractogram
 - DTR holds registered entries with assigned PIDs & information about the relationships for the data type, DIFFRACTOGRAM
 - EXAMPLE: RDA-Demo XRD Diffractogram 11314.3/c830042334b25fc6bc68 with multiple relationships identified
 - Based on query of DTR, NMRR can discover in MDCS & MDR
 - Relevant XRD diffractogram data sets
 - Data conversion resource to convert data into a plottable format
-
- Coarse vs. fine grain data types? **Coarse Data Types**
 - Resolvable unique id with relationships to other data types vs. natural language definition of the data type? **Resolvable ID**