Originally published in NISTIR 6785: MatML - Materials Markup Language Workshop Report

Please note that these examples illustrate the flexibility of MatML even if MatML is not yet optimized. The purposes of these examples are to provide informative illustrations for potential users of MatML and to uncover the strengths and weaknesses of the MatML Working Draft in order to formulate a plan for optimizing MatML and moving it forward to proposed recommendation status. (Example: Notice the information redundancy in the markup that must be addressed in a future version of MatML.)

The reader interested in the markup of complex materials systems such as composites is referred to Example 3.

Example 1: Structural ceramic from an online materials database
Source: “NIST WebSCD: http://www.ceramics.nist.gov/srd/scd/Z00363.htm,” R.G. Munro and E.F. Begley, 1998.

```
<?xml version="1.0"?>
<!--DOCTYPE MatML_Doc SYSTEM "MatMLv20.dtd"-->
<MatML_Doc>
<Material>
<BulkDetails>
<Name>silicon nitride</Name>
<Class>ceramic</Class>
<Specification>NCX-5102</Specification>
<Source>Saint-Gobain/Norton Industrial Ceramics
<Form>bar</Form>
<Processing>
<Name>hot isostatic pressing</Name>
<Notes>
"The material produced is designated NCX-5102 and consists of a silicon  nitride-4% yttria
composition that is densified by glass-encapsulation  HIPing. ... Large-scale batches (30 kg) of
Si<sub>3</sub>N<sub>4</sub>-4% Y<sub>2</sub>O<sub>3</sub> powder were  milled in
water,
and the slurry was used to cast hundreds of tensile rods. The starting
Si<sub>3</sub>N<sub>4</sub> powder (Ube) was derived from a dimmide process. ...  The net-
shape-formed bars were HIPed using glass encapsulation (ASEA Cerma  AB, Robertsford,
Sweden).  The HIP process was optimized using
pressure, time  and temperatures to assure full densification and development of an elongated
microstructure for desired fracture toughness..."
</Notes>
</Processing>
<Characterization>
<Formula>
Si<sub>3</sub>N<sub>4</sub>&#183;4wt%Y<sub>2</sub>O<sub>3</sub></Formula>
<ChemicalComposition>
<Compound>
<Element>Si</Element>
<Units>3</Units>
<Element>N</Element>
<Units>4</Units>
</Compound>
```

<Concentration>96</Concentration>
<Units>wt%</Units>
<Compound>
<Element>Y</Element>
<Units>2</Units>
<Element>O</Element>
<Units>3</Units>
</Compound>
<Concentration>4</Concentration>
<Units>wt%</Units>
<Notes>sintering aid</Notes>
</ChemicalComposition>
</Characterization>
<Properties>
<PropertyDetails>
<Name>Flexural Strength</Name>
<Units>MPa</Units>
<DataSource>Journal article
Title - Reliable Ceramics for Advanced Heat Engines
Author(s) - V.K. Pujari, D.M. Tracey, M.F. Foley, N.I. Paille, P.J. Pelletier, L.C. Sales, C.A. Willkens, and R.L. Yeckley
Publication - American Ceramic Society Bulletin
Volume - 74
Issue - 4
Year - 1995
Page(s) - 86-90
Publisher - American Ceramic Society
</DataSource>
<DataType>Evaluated</DataType>
<MeasurementTechnique>
<Name>Strength tests</Name>
<Notes>
The authors cite V.R. Pujari et al., "Development of Improved Processing and Evaluation Methods for High Reliability Structural Ceramics for Advanced Heat Engine Applications, Phase I," final report,
ORNL/Sub/89-SB182/1, NTIS Rept. No. DE93-040528, August (1993), and summarize the procedure as follows. "The cylindrical buttonhead specimens were machined to ORNL design with a gauge diameter of 6.0±0.1 mm. ...50 mm diameter, 150 mm long specimens... were machined as many flexure bars (3 mm by 4 mm by 50 mm) for assessment of the properties across the 50-mm section."
</Notes>
</MeasurementTechnique>
<Notes>
Cautions: Evaluated Data.
"The nonlinear character of the distribution with multiple inflections suggests that a two-parameter Weibull fit of these data (sigma = 1038 MPa, m = 10.4) is inappropriate and that the multimodal nature of the data should be represented using competing risk analysis. ... The important feature of the three-parameter Weibull distribution is the existence of a threshold stress below which there is zero probability of failure."
</Notes>
</PropertyDetails>

<Value type="integer">972,561</Value>
<Parameters>
<Name>Test Temperature</Name>
<Value type="integer">23,1370</Value>
<Units>°C</Units>
</Parameters>
<PropertyDetails>
<Name>Tensile Strength</Name>
<Units>MPa</Units>
<DataSource>Journal article
Title - Reliable Ceramics for Advanced Heat Engines
Author(s) - V.K. Pujari, D.M. Tracey, M.F. Foley, N.I. Paille, P.J. Pelletier, L.C. Sales, C.A. Willkens, and R.L. Yeckley
Publication - American Ceramic Society Bulletin
Volume - 74
Issue - 4
Year - 1995
Page(s) - 86-90
Publisher - American Ceramic Society
</DataSource>
<DataType>Evaluated</DataType>
<MeasurementTechnique>
<Name>Strength tests</Name>
<Notes>
The authors cite V.R. Pujari et al., "Development of Improved Processing and Evaluation Methods for High Reliability Structural Ceramics for Advanced Heat Engine Applications, Phase I," final report,
ORNL/Sub/89-SB182/1, NTIS Rept. No. DE93-040528, August (1993), and summarize the procedure as follows. "The cylindrical buttonhead specimens were machined to ORNL design with a gauge diameter of 6.0±0.1 mm. ...50 mm diameter, 150 mm long specimens... were machined as many flexure bars (3 mm by 4 mm by 50 mm) for assessment of the properties across the 50-mm section."
</Notes>
</MeasurementTechnique>
<Notes>
Cautions: Evaluated Data.
"The nonlinear character of the distribution with multiple inflections suggests that a two-parameter Weibull fit of these data (sigma = 1038 MPa, m = 10.4) is inappropriate and that the multimodal nature of the data should be represented using competing risk analysis. ... The important feature of the three-parameter Weibull distribution is the existence of a threshold stress below which there is zero probability of failure."
</Notes>
</PropertyDetails>
<Value type="integer">997,396</Value>
<Parameters>
<Name>Test Temperature</Name>
<Value type="integer">23,1370</Value>
<Units>°C</Units>
<Name>Range of Strengths</Name>
<Value type="text">540-1237,344-452</Value>
<Units>MPa</Units>

</Parameters>
<PropertyDetails>
<Name>Weibull Strength</Name>
<Units>MPa</Units>
<DataSource>Journal article
Title - Reliable Ceramics for Advanced Heat Engines
Author(s) - V.K. Pujari, D.M. Tracey, M.F. Foley, N.I. Paille, P.J. Pelletier, L.C. Sales, C.A. Willkens, and R.L. Yeckley
Publication - American Ceramic Society Bulletin
Volume - 74
Issue - 4
Year - 1995
Page(s) - 86-90
Publisher - American Ceramic Society
</DataSource>
<DataType>Evaluated</DataType>
<MeasurementTechnique>
<Name>Strength tests</Name>
<Notes>
The authors cite V.R. Pujari et al., "Development of Improved Processing and Evaluation Methods for High Reliability Structural Ceramics for Advanced Heat Engine Applications, Phase I," final report,
ORNL/Sub/89-SB182/1, NTIS Rept. No. DE93-040528, August (1993), and summarize the procedure as follows. "The cylindrical buttonhead specimens were machined to ORNL design with a gauge diameter of 6.0±0.1 mm. ...50 mm diameter, 150 mm long specimens... were machined as many flexure bars (3 mm by 4 mm by 50 mm) for assessment of the properties across the 50-mm section."
</Notes>
</MeasurementTechnique>
<Notes>
Cautions: Evaluated Data.
"The nonlinear character of the distribution with multiple inflections suggests that a two-parameter Weibull fit of these data (sigma = 1038 MPa, m = 10.4) is inappropriate and that the multimodal nature of the data should be represented using competing risk analysis. ... The important feature of the three-parameter Weibull distribution is the existence of a threshold stress below which there is zero probability of failure."
</Notes>
</PropertyDetails>
<Value type="integer">1109</Value>
<Parameters>
<Name>Test Temperature</Name>
<Value type="integer">23</Value>
<Units>°C</Units>
<Name>Weibull Modulus</Name>
<Value type="integer">4</Value>
<Units>none</Units>
<Name>Threshold Strength</Name>
<Value type="integer">665</Value>
<Units>MPa</Units>
</Parameters>
<PropertyDetails>

<Name>Weibull Modulus</Name>
<Units>none</Units>
<DataSource>Journal article
Title - Reliable Ceramics for Advanced Heat Engines
Author(s) - V.K. Pujari, D.M. Tracey, M.F. Foley, N.I. Paille, P.J. Pelletier, L.C. Sales, C.A. Willkens, and R.L. Yeckley
Publication - American Ceramic Society Bulletin
Volume - 74
Issue - 4
Year - 1995
Page(s) - 86-90
Publisher - American Ceramic Society
</DataSource>
<DataType>Evaluated</DataType>
<MeasurementTechnique>
<Name>Strength tests</Name>
<Notes>
The authors cite V.R. Pujari et al., "Development of Improved Processing and Evaluation Methods for High Reliability Structural Ceramics for Advanced Heat Engine Applications, Phase I," final report,
ORNL/Sub/89-SB182/1, NTIS Rept. No. DE93-040528, August (1993), and summarize the procedure as follows. "The cylindrical buttonhead specimens were machined to ORNL design with a gauge diameter of 6.0±0.1 mm. ...50 mm diameter, 150 mm long specimens... were machined as many flexure bars (3 mm by 4 mm by 50 mm) for assessment of the properties across the 50-mm section."
</Notes>
</MeasurementTechnique>
<Notes>
Cautions: Evaluated Data.
"The nonlinear character of the distribution with multiple inflections suggests that a two-parameter Weibull fit of these data (sigma = 1038 MPa, m = 10.4) is inappropriate and that the multimodal nature of the data should be represented using competing risk analysis. ... The important feature of the three-parameter Weibull distribution is the existence of a threshold stress below which there is zero probability of failure."
</Notes>
</PropertyDetails>
<Value type="text">4,---,---</Value>
<Parameters>
<Name>Stress Mode</Name>
<Value type="text">Tensile,Flexural,Flexural</Value>
<Units>none</Units>
<Name>Test Temperature</Name>
<Value type="integer">23,23,1370</Value>
<Units>°C</Units>
<Name>Threshold Strength</Name>
<Value type="integer">665,653,517</Value>
<Units>MPa</Units>
<Name>Weibull Strength</Name>
<Value type="text">1109,---,---</Value>
<Units>MPa</Units>
</Parameters>

</Properties>
</BulkDetails>
</Material>
</MatML_Doc>

Example 2: Aluminum alloy from a printed handbook
Source: Generously provided by F. Cverna of ASM International and J.G. Kaufman of the Aluminum Association from Properties of Aluminum Alloys, p. 291, ASM International, Materials Park, Ohio, ISBN: 0-87170-632-6, 1999.

```
<?xml version="1.0"?>
<!--DOCTYPE MatML_Doc SYSTEM "MatMLv20.dtd"-->
<MatML_Doc>
<Material>
<BulkDetails>
<Name>aluminum alloy</Name>
<Class>metal</Class>
<Specification>1350</Specification>
<Form>Rolled rod and shapes; smooth specimens</Form>
<Processing>
<Name>Temper</Name>
<Notes>H18</Notes>
</Processing>
<Properties>
<PropertyDetails>
<Name>Axial-Stress Fatigue Strength</Name>
<Units>ksi</Units>
<DataSource>
"Properties of aluminum alloys : tensile, creep, and fatigue data at high and low temperatures" /
edited by J. Gilbert Kaufman.
</DataSource>
<DataType>Handbook</DataType>
<Notes>Plus (+) indicates tension; minus (-) indicates compression.</Notes>
</PropertyDetails>
<Value type="float">+23,+17,+15,+14.5,+14.5</Value>
<Parameters>
<Name>Stress Ratio (R)</Name>
<Value type="integer">0,0,0,0,0</Value>
<Units>none</Units>
<Notes>Stress Ratio (R) = (minimum stress)/(maximum stress)</Notes>
<Name>Number of Samples</Name>
<Value type="integer">1,1,1,1,1</Value>
<Units>none</Units>
<Name>Number of Cycles</Name>
<Value type="integer">10^5,10^6,10^7,10^8,5x10^8</Value>
<Units>none</Units>
</Parameters>
<PropertyDetails>
<Name>Axial-Stress Fatigue Strength</Name>
<Units>MPa</Units>
<DataSource>
"Properties of aluminum alloys : tensile, creep, and fatigue data at high and low temperatures" /
edited by J. Gilbert Kaufman.
</DataSource>
<DataType>Handbook</DataType>
<Notes>Plus (+) indicates tension; minus (-) indicates compression.</Notes>
```

</PropertyDetails>
<Value type="integer">+160,+115,+105,+100,+100</Value>
<Parameters>
<Name>Stress Ratio (R)</Name>
<Value type="integer">0,0,0,0,0</Value>
<Units>none</Units>
<Name>Number of Samples</Name>
<Value type="integer">1,1,1,1,1</Value>
<Units>none</Units>
<Name>Number of Cycles</Name>
<Value type="integer">10^5,10^6,10^7,10^8,5x10^8</Value>
<Units>none</Units>
</Parameters>
<PropertyDetails>
<Name>Axial-Stress Fatigue Strength</Name>
<Units>ksi</Units>
<DataSource>
"Properties of aluminum alloys : tensile, creep, and fatigue data at high and low temperatures" / edited by J. Gilbert Kaufman.
</DataSource>
<DataType>Handbook</DataType>
<Notes>Plus (+) indicates tension; minus (-) indicates compression.</Notes>
</PropertyDetails>
<Value type="float">+11.5,+8.5,+7,+6.5,+6.5</Value>
<Parameters>
<Name>Stress Ratio (R)</Name>
<Value type="integer">-1,-1,-1,-1,-1</Value>
<Units>none</Units>
<Name>Number of Samples</Name>
<Value type="integer">1,1,1,1,1</Value>
<Units>none</Units>
<Name>Number of Cycles</Name>
<Value type="integer">10^5,10^6,10^7,10^8,5x10^8</Value>
<Units>none</Units>
</Parameters>
<PropertyDetails>
<Name>Axial-Stress Fatigue Strength</Name>
<Units>MPa</Units>
<DataSource>
"Properties of aluminum alloys : tensile, creep, and fatigue data at high and low temperatures" / edited by J. Gilbert Kaufman.
</DataSource>
<DataType>Handbook</DataType>
<Notes>Plus (+) indicates tension; minus (-) indicates compression.</Notes>
</PropertyDetails>
<Value type="float">+80,+59,+48,+45,+45</Value>
<Parameters>
<Name>Stress Ratio (R)</Name>
<Value type="integer">-1,-1,-1,-1,-1</Value>
<Units>none</Units>
<Name>Number of Samples</Name>

<Value type="integer">1,1,1,1,1</Value>
<Units>none</Units>
<Name>Number of Cycles</Name>
<Value type="integer">10^5,10^6,10^7,10^8,5x10^8</Value>
<Units>none</Units>
</Parameters>
</Properties>
</BulkDetails>
<Terms>
<termEntry>
<term>H18</term>
<definition>
"H18" is a code from The Aluminum Association Temper Designation System.
The H is defined as "strain-hardened (wrought products only). The 1 applies to products that are strain-hardened to obtain the desired strength without supplementary thermal treatment. The 8 indicates the degree of strain-hardening and is assigned to the hardest tempers normally produced.
</definition>
</termEntry>
<termEntry>
<term>1350</term>
<definition>
"1350" is a code from The Aluminum Association Alloy Designation System. The first digit of the code represents the principal alloying constitutent(s). The second digit indicates variations of the initial alloy. The third and fourth digits indicate individual alloy variations (the numbers have no significance but are unique). 1350 is an alloy that is pure AL (99.00% or greater). For further details, contact The Aluminum Association, 900 19th Street, N.W., Washington, D.C. 20006.
</definition>
</termEntry>
</Terms>
</Material>
</MatML_Doc>

Example 3: Steel with TiC coating from a journal article
Source: A. Agarwal and N.B. Dahotre, “Pulsed Electrode Surfacing of Steel With TiC Coating: Microstructure and Wear Properties,” ASM Journal of Materials Engineering and Performance, Vol. 8, No. 4, pp. 479-486, 1999.


```
<?xml version="1.0"?>
<!--DOCTYPE MatML_Doc SYSTEM "MatMLv20.dtd"-->
<MatML_Doc>
<Material>
<BulkDetails>
<Name>TiC coated AISI 1018 steel</Name>
<Class>composite</Class>
<Subclass>ceramic coating on metal substrate</Subclass>
<Form>coupon</Form>
<Properties>
<PropertyDetails>
<Name>Wear (Weight Loss Analysis)</Name>
<Units>g</Units>
<DataSource>
A. Agarwal and N.B. Dahotre, "Pulse Electrode Surfacing of Steel with TiC Coating:
Microstructure and Wear Properties," ASM Journal of Materials Engineering and Performance,
Vol. 8, No. 4, pp. 479-486, 1999
</DataSource>
<MeasurementTechnique>
<Name>Block-on-disk tribometer</Name>
<Notes>
"Coated coupons of dimension 25 x 25mm were tested for dry sliding wear against a hardened
steel ring rotating at a linear speed of 270m/min. Weight loss measurements were made after
successive 2
min. The dry sliding wear test was conducted for 10 min with an applied normal load of 2 kg."
</Notes>
</MeasurementTechnique>
<Notes>
Data were digitized from Fig. 9. The reported unit, "gm", is interpreted to mean "g", grams.
</Notes>
</PropertyDetails>
<Value type="float">.0011,.0018,.0023,.0027,.0029</Value>
<Parameters>
<Name>Time</Name>
<Value type="integer">2,4,6,8,10</Value>
<Units>minutes</Units>
<Name>Sliding Speed (Steel Ring)</Name>
<Value type="integer">270,270,270,270,270</Value>
<Units>m/minute</Units>
<Notes>See details in MeasurementTechnique Notes.       </Notes>
<Name>Applied Normal Load</Name>
<Value type="integer">2,2,2,2,2</Value>
<Units>kg</Units>
</Parameters>
<PropertyDetails>
<Name>Coefficient of Friction</Name>
```

<Units>none</Units>
<DataSource>See DataSource under Wear (Weight Loss Analysis)</DataSource>
<MeasurementTechnique>
<Name>Block-on-disk tribometer</Name>
<Notes>
"The coefficient of friction (μ) was also recorded simultaneously by an interface computer, which acquired data in the form of electrical output power of the motor. Even though data were recorded at a frequency of 1 Hz for a total test time of 10 min, an average of 10 successive points was taken for computing the coefficient of friction, μ. ...the coefficient of friction is calculated by measuring the changes in voltage and
current in the electrical circuit of the motor driving the block-on-ring tribometer during loading... "
</Notes>
</MeasurementTechnique>
</PropertyDetails>
<Value type="float">0.58</Value>
</Properties>
</BulkDetails>
<ComponentDetails>
<Name>steel</Name>
<Class>metal</Class>
<Specification authority="American Iron and Steel Institute">AISI 1018</Specification>
<Form>coupon</Form>
<Processing>
<Name>Mechanical polishing</Name>
<Notes> The coupons were mechanically polished on emery paper of grit size 240.</Notes>
<Name>Rinsing</Name>
<Notes> After polishing, the coupons were rinsed in acetone.</Notes>
<Name>Coating</Name>
<Notes>
"A sintered electrode of TiC was used to deposit a coating on these steel coupons. The TiC electrode had 3 to 5 wt% Ni and 1 to 3 wt% Fe as binder. Deposition was carried out using a handheld gun in air at room temperature. Pulsed electrode deposition was carried out at a voltage of 50V and spark time of 10μs. The discharge capacitance used for the PES process was 450μF with a current of 25A."
</Notes>
</Processing>
<Geometry>
<Shape>square</Shape>
<Dimensions>25mm x 25mm</Dimensions>
</Geometry>
<Properties>
<PropertyDetails>
<Name>Wear (Weight Loss Analysis)</Name>
<Units>g</Units>
<DataSource>See DataSource under Wear (Weight Loss Analysis) in BulkDetails.</DataSource>
<MeasurementTechnique>
<Name>Block-on-disk tribometer</Name>
</MeasurementTechnique>
<Notes> See Notes under Wear (Weight Loss Analysis) in BulkDetails.</Notes>

</PropertyDetails>
<Value type="float">.0019,.0036,.0057,.0073,.0090</Value>
<Parameters>
<Name>Time</Name>
<Value type="integer">2,4,6,8,10</Value>
<Units>minutes</Units>
<Name>Sliding Speed (Steel Ring)</Name>
<Value type="integer">270,270,270,270,270</Value>
<Units>m/minute</Units>
<Name>Applied Normal Load</Name>
<Value type="integer">2,2,2,2,2</Value>
<Units>kg</Units>
</Parameters>
<PropertyDetails>
<Name>Microhardness</Name>
<Units>kg/mm^2</Units>
<MeasurementTechnique>
<Name>Knoop Indentation</Name>
<Notes>
"Microhardness measurements were performed on a Buehler Micromet II microhardness tester using a Knoop indenter with normal load of 200 g applied for 15 s."
</Notes>
</MeasurementTechnique>
</PropertyDetails>
<Value type="text">172 ± 12</Value>
</Properties>
<Associations>
<Associate>titanium carbide coating</Associate>
<Relationship>substrate</Relationship>
</Associations>
<Name>titanium carbide coating</Name>
<Class>carbide</Class>
<Subclass>monocarbide</Subclass>
<Characterization>
<Formula>TiC· xFe</Formula>
<PhaseComposition>
<Name>TiC</Name>
<Concentration type="text">Not reported</Concentration>
<Units>Not applicable</Units>
<Name>Ti</Name>
<Concentration type="text">5 - 25</Concentration>
<Units>wt%</Units>
<Name>Fe-C (austenite)</Name>
<Concentration type="text">Not reported</Concentration>
<Units>Not applicable</Units>
<Name>Fe (ferrite)</Name>
<Concentration type="text">Not reported</Concentration>
<Units>Not applicable</Units>
<Name>FeTi</Name>
<Concentration type="text">Not reported</Concentration>
<Units>Not applicable</Units>

<Qualifier>Possible</Qualifier>
</PhaseComposition>
</Characterization>
<Properties>
<PropertyDetails>
<Name>Microhardness</Name>
<Units>kg/mm^2</Units>
<MeasurementTechnique>
<Name>Knoop Indentation</Name>
<Notes> See MeasurementTechnique Notes for Microhardness in the steel component.</Notes>
</MeasurementTechnique>
</PropertyDetails>
<Value type="text">1235 ± 86</Value>
</Properties>
<Associations>
<Associate>AISI 1018 steel</Associate>
<Relationship>coating</Relationship>
</Associations>
<Name>Heat Affected Zone (HAZ)</Name>
<Properties>
<PropertyDetails>
<Name>Microhardness</Name>
<Units>kg/mm^2</Units>
<MeasurementTechnique>
<Name>Knoop Indentation</Name>
<Notes> See MeasurementTechnique Notes for Microhardness in the steel component.</Notes>
</MeasurementTechnique>
</PropertyDetails>
<Value type="text">352 ± 32</Value>
</Properties>
<Notes>Martensitic zone</Notes>
</ComponentDetails>
</Material>
</MatML_Doc>