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3D PRINTED MODELS OF MATERIALS TENSOR REPRESENTATIONS AND THE CRYSTAL MORPHOLOGY OF ALPHA QUARTZ

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Abstract: The Materials Property Open Database (MPOD) is a unique open-access resource for Materials Physics research and education. Longitudinal materials tensor representation surfaces for selected physical properties of alpha-quartz crystals, (i.e. its elastic stiffness and piezoelectric effect) were visualized at the MOPD website and corresponding 3D print files created automatically by a simple click of the computer mouse. The usage of the Windows™ executable program Wintensor™ is presented as an alternative to this kind of workflow in cases where the corresponding data are not (yet) in this database, where more control over the creation of the print files and 3D printing in two colors are desired for representation surface parts with positive and negative signs, e. g. those for optical activity (rotational power) and the linear electro-optical (Pockels) effect in α-quartz. In accordance with Franz Ernst Neumann's principle, restrictions on the number of the independent materials tensor components for the above mentioned physical properties by the point symmetry of α-quartz and the nature of the involved field tensors are explicitly mentioned. An appendix illustrates the crystal morphology of right α-quartz.

Keywords: Materials physics, open-access databases, tensors, longitudinal representation surfaces, 3D printed models, Neumann's symmetry principle.

While 3D printing has been available for more than a quarter of a century, cost and performance improvements have only recently made it practical for usage by researchers and educators to create handouts of crystallographic models of various kinds (Casas and Estop, Chakraborty and Zuckermann, Chen et al., Flint, Gražulis et al. 2015, Herman et al., Kaminsky et al., Kitson et al., Meyer, Moeck et al., Olson et al., Rodenbough et al., Rossi et al., Scalfani and Vaid, Snyder et al., Stone-Sundberg et al., and Wedler et al.). The 3D printing process requires files in the industry-wide accepted Standard Tessellation Language (STL, file extension *.stl, for single color print outs) or Virtual Reality Modeling Language (VRML, file extension *.wrl, for print outs in more than one color) format. Detailed information on Materials Physics is way beyond the scope of this paper. The reader is referred to popular college level textbooks (Haussühl, Newnham, Nye, Paufler, Zolotoyabko) when such information is sought.

A French-Mexican collaborative team (Fuentes-Cobas et al.) offers the creation to monochrome 3D print files of longitudinal representation surfaces of physical properties of crystals together with their on-line visualizations at the websites of their Material Properties Open Database (MPOD) at Caen, France (Pepponi et al.) and its mirror in Mexico (http://mpod.cimav.edu.mx/). The MPOD is a unique resource for Materials Physics research and education and its creation was inspired by the great success of the Crystallography Open Database, COD (Gražulis et al. 2009 and 2011), which provides currently open access to more than 360,000 entries on small molecules and small to medium sized unit cell crystals (including minerals - as it contains all of the entries of the American Mineralogist Crystal Structure Database (http://rruff.geo.arizona.edu/AMS/amcsd.php, AMCSD, Downs and Hall-Wallace) - but excluding biopolymers). The data entries of the COD are in the very versatile and well documented (see Volume G of the International Tables for Crystallography, edited by Hall and McMahon) Crystallographic Information Framework (CIF, *.cif) file format (Hall et al., Bernstein et al.) as endorsed by the International Union of Crystallography.

The CIF format itself is based on the STAR format (Hall, Spadaccini and Hall) and the developers of the MPOD utilized the STAR format for the comprehensive representation of their own data, see, e.g. Fig. 1. This resulted in human beings being able to comprehend the data entries directly. The complementing purpose-written dictionary (as integral part of the STAR inspired format) may need to be consulted for more details and perhaps in order to be sure that the physical units of the tensor components are given according to the Système International d'unités, SI, (rather than

the British Imperial or the United States Customary systems). Obviously, having all entries in a STAR format compatible syntax and supported by a dictionary enables computerized data checking and handling, just as this is the case for the corresponding atomistic structure entries in the *.cif format from the COD and AMCSD.

Figure 1 displays a browser screen shot for a successful search for physical data on crystalline quartz in its low temperature, alpha, phase modification. Data entries such as 'RUS' (for Resonance Ultrasonic Spectroscopy) in this figure are explained in the syntax dictionary that can also be assessed directly at the MPOD website. The inset (on yellow background) in Fig. 1 shows the content of a unit cell of a left α-quartz crystal together with its space group and unit cell parameters. Interactive visual representations such as the latter are openly accessible at the website of the COD (www.crystallography.net), at its various mirrors, and at the AMCSD website. The corresponding data file of the COD is 1526860.cif. Taken together, the COD, AMCSD, and MPOD provide comprehensive information on the structure and physical properties of crystalline materials.

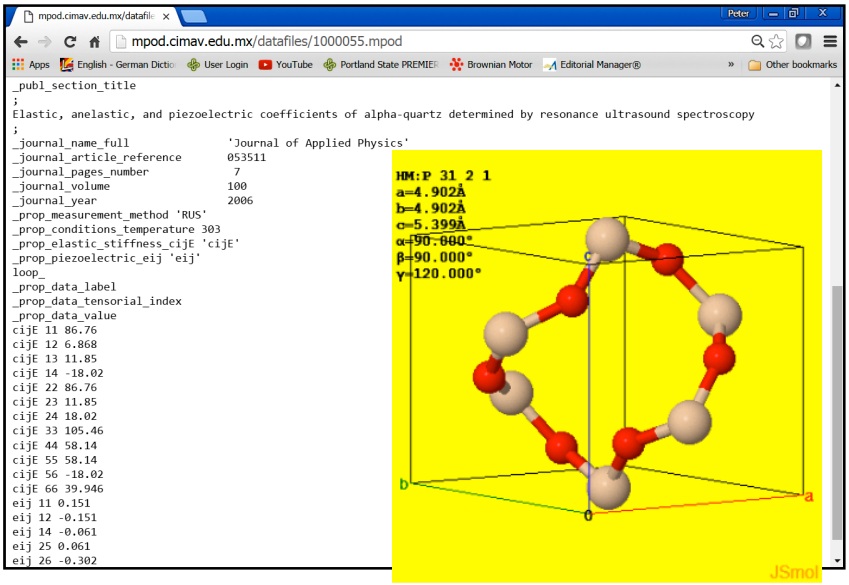

Figure 1: Screen shot of selected physical properties of α-quartz in a STAR syntax compliant file from the MPOD. A JSmol display of the corresponding crystal structure (form the COD) acts as a complementing inset. The inset shows the symmetry equivalent positions within one unit cell of left α-quartz with Si^{+4} at (0.4673, 0, 0.3333) in Wyckoff position 3a, and O^{-2} at (0.413, 0.2711, 0.2172) in Wyckoff position 6c, from the COD file 1526860.cif together with the crystal's space group ($P3_12$) and unit cell parameters.

Space group $P3_12$ of left[1] (leavorotative) α-quartz (as mentioned in the inset in Fig. 1) corresponds to point group 32. According to Neumann's principle ***"the symmetry operations of any physical property of a crystal must include the symmetry operations of the point group of the crystal"*** (http://reference.iucr.org/dictionary/Neumann's_ principle), this point group reduces the number of independent tensor coefficients for the elastic stiffness (which is a 4th rank tensor) to six and for the piezoelectric effect (which is a 3rd rank tensor) to two, respectively. Figure 1 lists a total of 12 and 5 components for these two polar tensors in matrix form. (Obviously only six and two of these components are independent.) All not explicitly mentioned components of the corresponding 6 by 6 and 3 by 6 matrices are zero. The information in data files from the MPOD can, thus, directly be taken to write down the respective matrices.

At the second page of a successful search for a crystal phase in the MPOD, see e.g. Figs. 2a and 2b, matrix representations of the physical properties are given explicitly so that the user does not necessarily need to open the corresponding *.mpod data file (as shown opened up in Fig. 1). At MPOD pages such as shown in Figs. 2a and 2b, the user can view longitudinal representation surfaces of the materials tensors and apply different color schemes to the display in order to highlight certain aspects. Most importantly in the context of this paper, the user can produce the corresponding 3D print files with a click of the computer mouse.

Figures 2a and 2b visualize three physical properties of α-quartz, i.e. elastic compliance and stiffness (Young modulus) as well as piezoelectricity in correspondence to the data in MPOD file 1000055.mpod. In such 3D visualizations, the magnitude of the physical property is given by the radial vector magnitude of a given surface point from the origin of the reference frame. The anisotropy of a physical property is represented by the angular variation of the corresponding longitudinal representation surface. (A sphere would have now such variation and, hence, represent an isotropic physical property.)

Figure 2a visualizes both the elastic compliance and stiffness tensor of α-quartz. The default "jet" color code has been applied. Color coding of longitudinal representation

[1] Left refers here to the position of usually rather small trigonal dipyramid $\{2h\bar{h}\bar{h}l\}$ and trigonal trapezohedron $\{hkil\}$ faces on the typically well-developed hexagonal prism $\{10\bar{1}0\}$ faces of α-quartz crystals while looking upwards along the crystallographic ***c***-axis (which is parallel to the Crystal Physics z-axis). The distinction between the two enantiomorph α-quartz crystal morphologies is further elaborated on in the appendix.

surfaces of the respective materials tensors is not really necessary, but may facilitate the direct numerical appreciation of the magnitude of the physical property in connection with the color explaining legend. Note the reciprocity relationship between the two representation surfaces in Fig. 2a, which is particularly nicely revealed by the chosen color coding scheme.

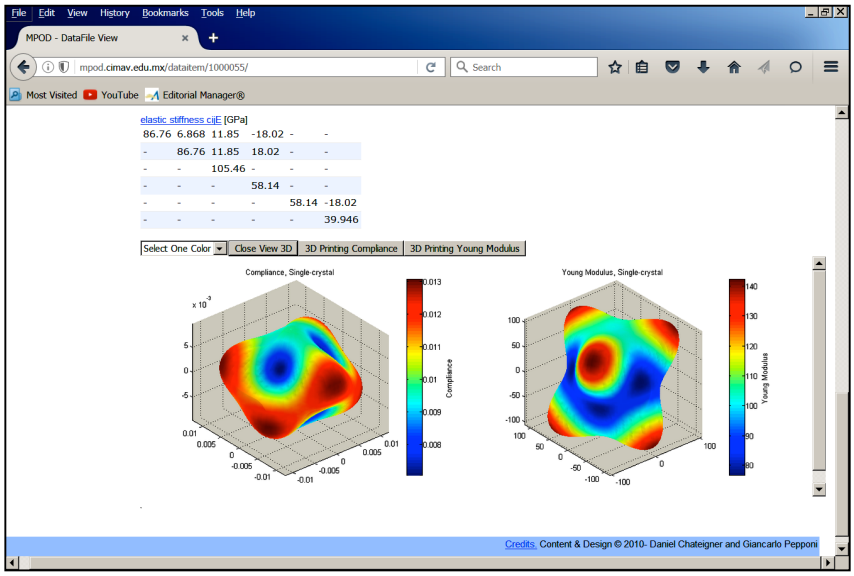

Figure 2a: Bottom part of a page of the MPOD that gives an overview of the results of an experimental measurement of the elastic properties of α-quartz. The physical unit of the matrix components of the elastic stiffness tensor (Young's modulus, right) is Giga-Pascal.

Figure 2b visualizes the longitudinal piezoelectric effect tensor in α-quartz. In this case, the non-default 'gray scale' visualization was chosen. As already mentioned, 3D print files can be produced directly at the website of the MPOD by clicking on the respective display buttons. The resulting files are in the *.stl format, which allows for monochrome model printing only (as mentioned further above). Monochrome 3D printing suffices for the longitudinal representation surfaces of the elastic stiffness and piezoelectricity as these two physical properties have positive signs everywhere. Figure 3 shows the corresponding 3D print outs.

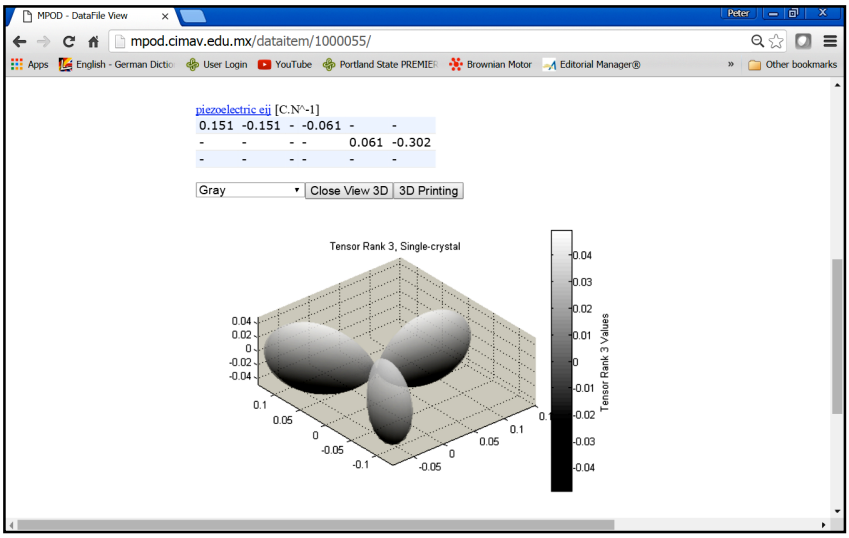

Figure 2b: Part of a page of the MPOD that gives an overview of the piezoelectric properties of α-quartz. The corresponding MPOD data file, 1000055.mpod - as opened up in Fig. 1, also gives the temperature of the measurement (303 K) because the effect is strongly dependent on it (and disappears at 846 K with the phase transition to beta-quartz). The physical unit of the tensor components is Coulomb per Newton.

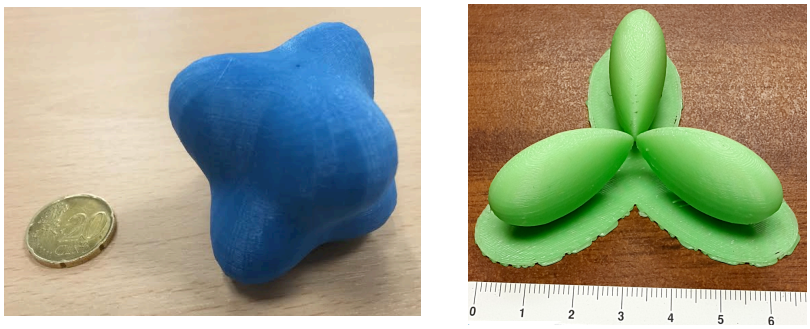

Figure 3: 3D print outs of the longitudinal representation surfaces of the elastic stiffness (left) and the piezoelectric effect (right) in α-quartz. A European 20 cent coin and a centimeter ruler provide indications of the size of these models. In the model on the right hand side, an extra support has been added during the printing process in order to stabilize it at its center.

3D prints of longitudinal representation surfaces for the rotational power (optical activity) and the linear electro-optical (Pockels) effect of α-quartz, on the other hand,

benefit enormously from color printing (on the basis of the *.wrl format) because their physical property anisotropy visualizations involve regions with positive and negative signs.

Werner Kaminsky's Wintensor™ program (http://cad4.cpac.washington.edu/WinTensorhome/WinTensor.htm) can be utilize for the creation of the corresponding color information containing 3D print files. Figure 4 shows a screen shot of this program that displays the rotational power (optical activity) in α-quartz. The corresponding (second rank) axial pseudo-tensor possesses two independent components. Note that versions of Wintensor™ have been around for more than 15 years (Kaminsky 2000).

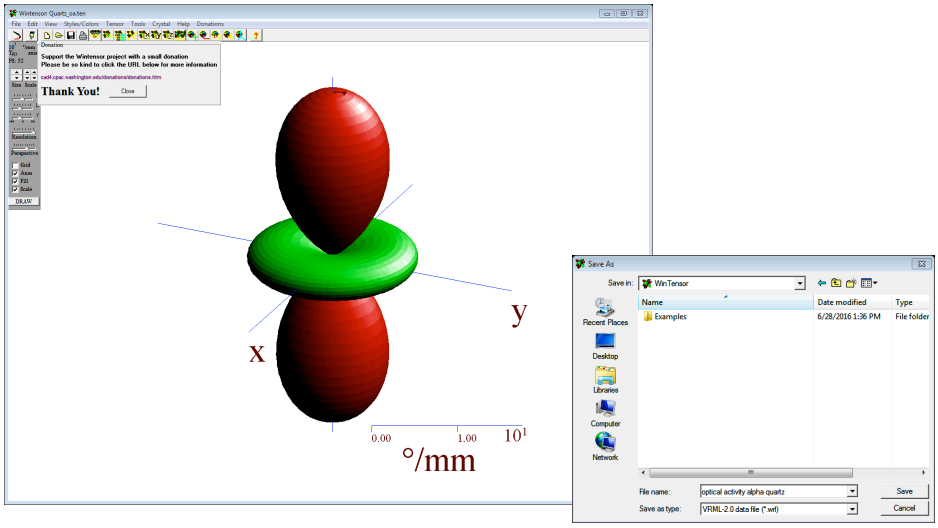

Figure 4: Screenshot of the Wintensor™ program displaying the longitudinal representation surface of the rotational power (optical activity) of α-quartz. The monochrome point group of the physical property is ∞ 2, which allows for clockwise and anticlockwise rotations and is a supergroup of 32. The user can choose to convert the displayed model to either the *.stl or the *.wrl format, as documented by the inset to the right.

For right (dextrorotative) α-quartz, space group $P3_22$, the red color in the visualization of Fig. 4 and the 3D model that has been printed from a *.wrl file, Fig. 5, corresponds to a clockwise rotation of linearly polarized light (when looking towards the light source through the sample). The green color corresponds to an anticlockwise rotation. For a left α-quartz crystal, space group $P3_12$, the rotation directions are reversed. The discussed

polar materials tensors (of forth and third rank) mentioned above and visualized in Figs. 2a and 2b, on the other hand, do not have any "rotation directionality", i.e. have the same longitudinal representation surfaces for left and right α-quartz. A 3D printed model of the representation surface of optical activity (rotational power) of α-quartz is shown together with a 3D printed model of the crystal's morphology in Figure 5. The morphology model refers to a right α-quartz crystal, see appendix for more details.

The corresponding *.stl print file for the crystal morphology model was created with the current version of Werner Kaminsky's WinXmorph™ (http://cad4.cpac.washington.edu/WinXMorphHome/WinXMorph.htm) program (Kaminsky 2005 and 2007). This program has been around for more than 15 years as well and allows since 2007 for the utilization of crystal morphology information in the above mentioned *.cif format.

Figure 5: 3D printed models of the rotational power (optical activity) of α-quartz (left) and the crystal's morphology (right) in the hands of the worldly Office Administrator of the Department of Physics of Portland State University. (She holds the crystal morphology model of a right α-quartz in her right hand.)

The left hand side of Figure 6 shows a part of the screenshot of the Wintensor™ program that displays the linear electro-optical (Pockels) effect in α-quartz. As another example of a third rank polar tensor, this effect is described in this crystal by two independent components. A photograph of the corresponding printed out model of the two-color longitudinal representation surface is shown on the right hand side of this

Figure. Surface parts in red color refer to changes in the refractive index that increase its value and the green color represents decreases of this dimensionless property in Fig. 6.

Finally, we like to mention that Werner Kaminsky created recently the program Cif2VRML (http://cad4.cpac.washington.edu/WinXMorphHome/Cif2VRMLHome/Cif2VRML.htm) for the direct conversion of atomic level molecule and crystal structure information from the *.cif format (as available in open access from the COD and AMCSD, for additional sources of CIFs see a recent review by Glasser) to the *.stl and *.wrl 3D print file formats (Kaminsky et al. 2014). Files that were created with this program are available for free downloads at Portland State University's Open Access Crystallography website (http://nanocrystallography.research. pdx.edu).

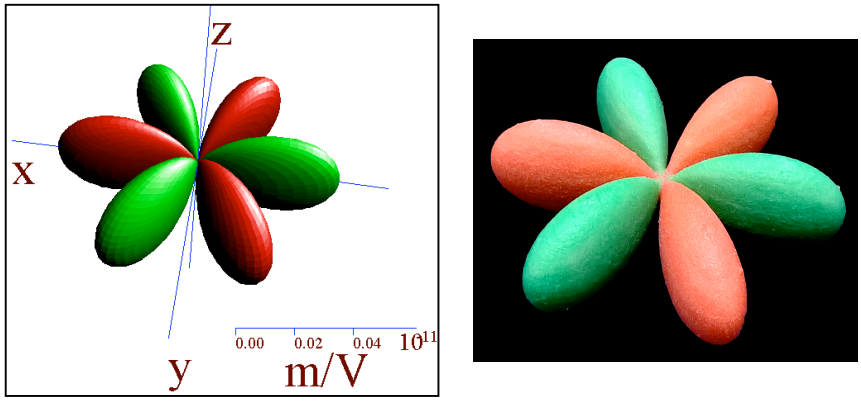

Figure 6: Longitudinal representation surface of the linear electro-optical (Pockels) effect in α-quartz (left) as cropped from a screenshot of the Wintensor™ program and the corresponding 3D print out (right). The size of the 3D printed model is such that the 3.3 cm length of any one of the three positive (green) and three negative (red) lobes corresponds to 0.48 pm/V.

In summary, this paper informs the readers of *Symmetry: Culture and Science* about recent developments around the 3D printing of crystallographic models. We mentioned Neumann's symmetry principle, provided the number of independent tensor components for the physical properties of α-quartz that we discussed, and leave it as a challenge to astute readers of this journal to verify these numbers independently. Note also that all of the visualized and 3D printed materials tensor representation surfaces possess symmetries that contain the point symmetry of α-quartz in accordance with Neumann's

principle. The crystal morphology model, see appendix, possesses of course the point group of α-quartz (while not being a tensor property).

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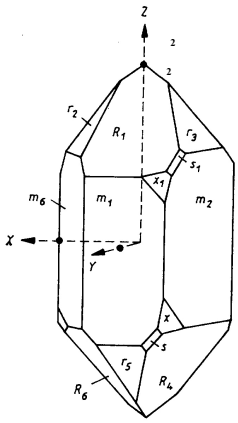
Appendix: Sketch of the typical morphology of right α-quartz crystals



$m_1 = (01\bar{1}0)$; m_2 and m_6 symmetry related $\{10\bar{1}0\}$

$R_1 = (01\bar{1}1)$; R_4 and R_6 symmetry related $\{0k\bar{k}l\}$

$r_2 = (10\bar{1}1)$; r_3 and r_5 symmetry related $\{h0\bar{h}l\}$

$s_1 = (\bar{1}2\bar{1}1)$; s_2 symmetry related $\{hh2\bar{h}l\}$

$x_1 = (\bar{1}6\bar{5}1)$; x_2 symmetry related $\{hkil\}$

The position of the faces s_1 and x_1 with respect to face m_1 make it clear that this is a sketch of a right α-quartz. (Corresponding faces would be located on the left hand of face m_1 in left α-quartz.) An orthogonal right-handed Crystal Physics coordinate system ($\boldsymbol{X}//\boldsymbol{a_1}$) is drawn in. Modified after a similar sketch in Paufler, P. (1986) *Physikalische Kristallographie*, Akademie-Verlag, Berlin.