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Sandia National Laboratories

Evaluating the ~~Temperature~~ Pressure Dependence of PZT Structures Using a Virtual Reality Environment

PRESENTED BY

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U.S. DEPARTMENT OF ENERGY NNSA

Success was facilitated by a scientifically diverse team with many contributors

Team:

Mark Rodriguez	– Project Coordinator
John Krukar	– Lead Virtual Reality Programmer
Zach Harris	– Support Virtual Reality Programmer
Nichole Valdez	– Crystallography & CIF Support
Kathryn Perkins	– PZT Materials Subject Matter Expert
Chris DiAntonio	– Funding support & PZT Subject Matter Expert
Pin Yang	– PZT Subject Matter Expert

Mark's contribution

"If you're referring to the incident with the Dragon, I was barely involved. All I did was give your uncle a little nudge out of the door."— J.R.R. Tolkien

The Fellowship of the Ring
Peter Jackson Director

We wanted to build a Virtual Reality tool to enable ***intuitive*** evaluation of crystal structures

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Pressure-induced ferroelectric to antiferroelectric phase transition in $Pb_{0.99}(Zr_{0.95}Ti_{0.05})_{0.98}Nb_{0.02}O_3$

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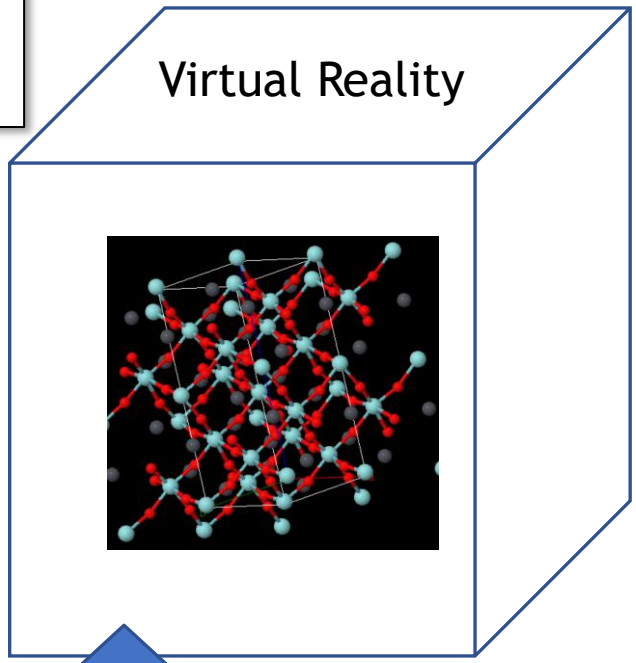
How can I take this…

P (kbar)	0	1.7	2.1	6.2
a (Å)	5.84858(7)	5.84513(6)	5.8440(4)	5.8383(13)
c (Å)	14.4230(3)	14.4074(3)	14.400(1)	14.368(6)
z(Pb)	0.2825(2)	0.2819(1)	0.2815(5)	0.273(3)
U_{11}(Pb)(Å^2)	0.0193(6)	0.0173(5)	0.0173(—)	0.0173(—)
U_{33}(Pb)(Å^2)	0.0084(8)	0.0082(7)	0.0082(—)	0.0082(—)
z(Zr/Ti)	0.0128(2)	0.0125(2)	0.0129(6)	0.036(3)
U_{iso}(Zr/Ti)(Å^2)	0.0061(3)	0.0068(3)	0.0068(—)	0.0068(—)
x(O)	0.1426(3)	0.1408(3)	0.1483(12)	0.172(5)
y(O)	0.3473(3)	0.3473(3)	0.3573(10)	0.389(4)
U_{11}(O)(Å^2)	0.0188(10)	0.0182(9)	0.0182(—)	0.0182(—)
U_{22}(O)(Å^2)	0.0105(8)	0.0112(8)	0.0112(—)	0.0112(—)
U_{33}(O)(Å^2)	0.020(1)	0.021(1)	0.021(—)	0.021(—)
U_{12}(O)(Å^2)	0.0049(11)	0.0062(10)	0.0062(—)	0.0062(—)
U_{13}(O)(Å^2)	−0.0015(10)	−0.0011(9)	−0.0011(—)	−0.0011(—)
U_{23}(O)(Å^2)	−0.0063(6)	−0.0056(6)	−0.0056(—)	−0.0056(—)
R_p (%)	3.94	3.57	3.33	4.01
R_{wp} (%)	6.65	5.81	5.13	6.45
χ^2	1.52	1.53	2.36	1.49

…and seamlessly import it into a 3D virtual reality?



CIF file

OpenBabel CIF reader

John Krukar and Zach Harris will give us a tour of the new CrystalVR Visualization tool

\\snl\collaborative\Xraydata\PZT_visualization

Thank you!

Questions?

https://CAD2VR.sandia.gov

Acknowledgment:

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