

Embedded and Interactive 3D Graphics for Materials Science

Jonathan D. Emery

Lecturer
Materials Science and Engineering
Northwestern University

August 17th, 2018

Outline

1. Learning in 3D Space
 - 1.1 Background
 - 1.2 Interactive 3D Graphics as a Learning Tool

2. Asymptote + PDF
 - 2.1 The Decision
 - 2.2 Gallery
 - 2.3 Successes
 - 2.4 Challenges

3. Afterward — HTML5-embeddable 3D Content

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Acknowledgments and Resources

Funding from Northwestern University's Digital Learning Fellowship

GitHub repository: <https://github.com/emeryjdk/NAMES-2018>

- ▶ Asymptote Script (.asy)
- ▶ 3D PDFs (.pdf)
- ▶ Jupyter Notebooks (.ipynb)
- ▶ Interactive HTML Snippets (.html)

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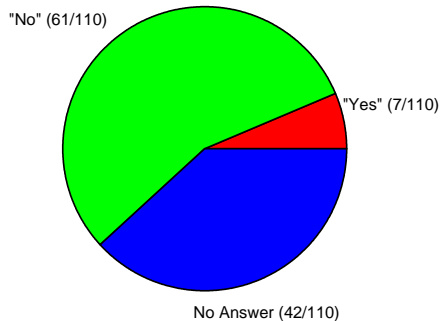
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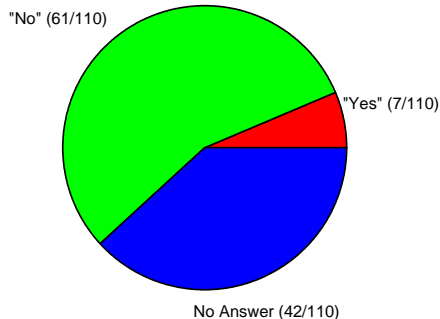
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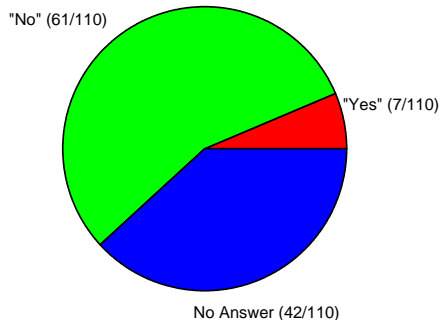
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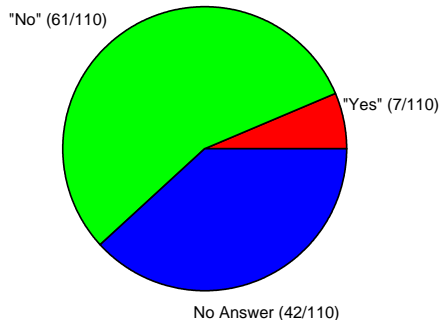
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“Cumbersome”

“Didn’t want to learn software” / “No time”

Visualization Software for MSE

Topic	Example Software
Math (vector fields, energy surfaces)	<u>Mathematica</u> , <u>MATLAB</u> , Python
Crystallography/Polymers/Molecules	<u>CrystalMaker</u> , <u>VESTA</u> , OVITO, <u>JSMol</u> , CrystalWalk
Defects/Imperfections	<u>CrystalMaker</u> , OVITO
Phase Diagrams	<u>ThermoCalc</u> , <u>JMol</u>
Microscopy/Microstructure	<u>Paraview</u> , <u>ImageJ</u>
Electronic Structure/Band Structure	Vesta, MATLAB, QuantumATK
CAD/FEM/3D Printing	AutoCAD, SolidWorks, SketchUp, <u>COMSOL</u>
Materials Selection	<u>CES Edupack</u> (in 3D?)

Underlined: Software used at some point in our curriculum.

Boxed Software that enables most of our 3D visualization goals.

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Do 3D and Interactive Graphics Help?

Should I even bother?

Höffler, University of Kiel, Olshausenstr —

Spatial Ability: It's Influence on Learning with Visualizations — a Meta-Analytic Review

Educ. Psychol. Rev. (2010) 22:245-269

	Low-level Spatial Ability Learners Enhance (Compensate)	High-Level Spatial Ability Learners Enhance
Dynamics	High (Yes)	Medium
Dimensionality	High (Yes)	Medium
Realism	Medium (No)	Medium
Interactivity	Medium (No)	Medium
Multi-modal	Low (No)	Low

Conclusion → Yes, with focus. Need to:

- ▶ Reduce student barriers to access 3D models.
- ▶ Streamline visualization features to provide resources for various learners.

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One-stop-shop Visualization

Can I put sophisticated 3D visualizations directly into my students' course documents?

Considerations:

Idealalities :

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Considerations:

- ▶ Free/cheap
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Idealalities :

- ▶ Interactivity
- ▶ Active/responsive development community
- ▶ Virtual reality
- ▶ Data collection

Goals for Project

- ▶ Increase participation in utilizing 3D graphics.
- ▶ Improve student outcomes in areas that hinge on visualization of complex 3D structures.
- ▶ Improve student satisfaction with course materials through well-integrated and easy-to-use content.
- ▶ Establish a platform to easily deployment complex 3D data for richer data communication.
- ▶ Better understand how students use and interact with these graphics.
- ▶ **Impress my students.**

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Asymptote + PDF (Adobe)

Asymptote — Vector Graphics Software (John Bowman, U. of Alberta)

- ▶ PDF formatting are a ubiquitous medium for course documentation and journal publications
- ▶ *Asymptote* compiles through T_EXnicCenter
- ▶ *Asymptote* → PRC (Product Representation Compact)
 - ▶ Powerful vector graphics language
 - ▶ High-level graphics commands (flexibility)
 - ▶ T_EX-formatted labeling
 - ▶ PRC files are ISO-standardized
 - ▶ Viewable with Adobe Reader*
 - ▶ JavaScript-enabled views, animations, and interactivity

*We'll talk about this in a bit...

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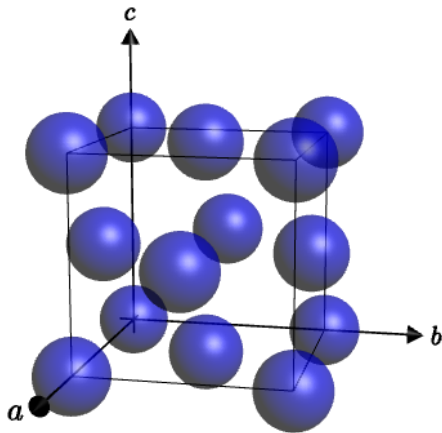
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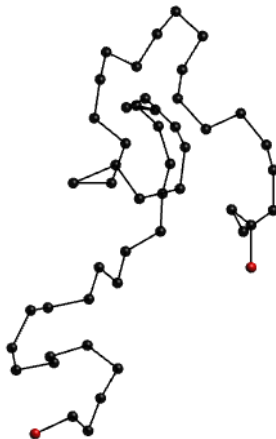
The FCC Crystal Structure



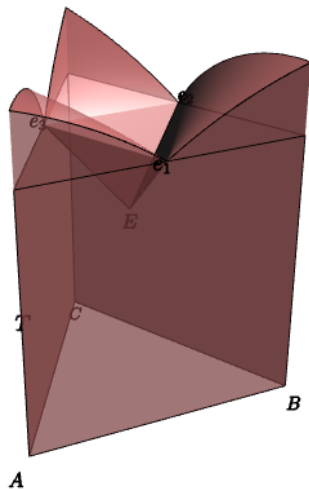
How many octahedral sites are there in this unit cell?

Rotate the crystal to view along the $[111]$ direction.

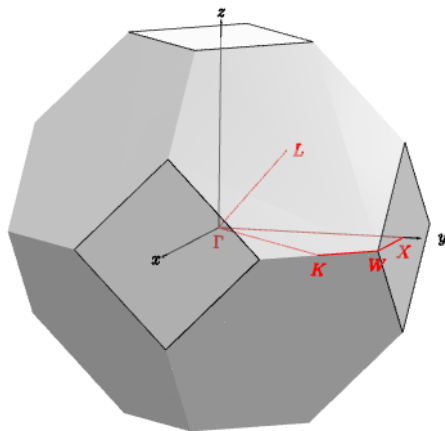
Polymer Random Walk



Ternary Phase Diagram (extra fresh)



Brillouin Zone[†]



[†]From StackExchange users dasausTeR and cfr

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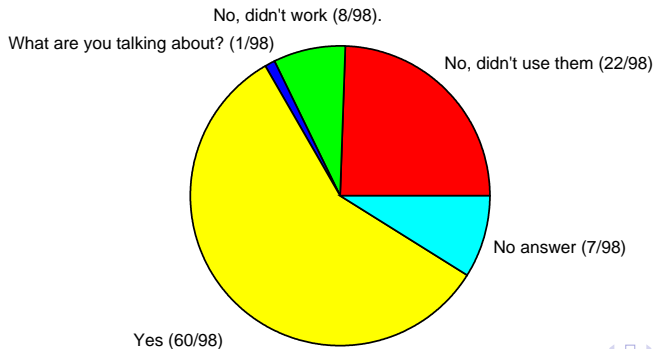
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- ▶ Collaborative — join on GitHub!
- ▶ Paste into your PDF from my PDF



Challenges

- ▶ ~10% of students can't follow a one-step direction to download Adobe.
- ▶ Adobe is no longer the *de facto* PDF-viewer
- ▶ Creation is complex...
- ▶ User-end settings and hardware:
 - ▶ No tablets
 - ▶ No phone
 - ▶ Loading time
 - ▶ Securities
 - ▶ Adobe!
- ▶ It does not work *directly* with PowerPoint (but nothing does, really...)
- ▶ Is our children learning?

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Need a better option — something for the web —

- ▶ Our students *live* on the Web.
- ▶ Something *simpler*.
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