

## VESTA Exercise sheet A

### Crystal structure of diamond and graphite.

1. Download (and install) the soft-wave program VESTA from the web.  
<http://jp-minerals.org/vesta/en/download.html>
2. Find and download the diamond and graphite VESTA files from:  
[http://www.misasa.okayama-u.ac.jp/~masami/pukiwiki/index.php?Vesta\\_data](http://www.misasa.okayama-u.ac.jp/~masami/pukiwiki/index.php?Vesta_data)
3. Open the downloaded files with VESTA.
4. Which atoms are diamond and graphite made of?
5. Try the following on diamond. Click on the "properties"-button -> "Single unit cell".
6. For clarity: click on "Edit" -> "Bonds" -> click on the row where the atoms are -> click on "Do not search atoms beyond the boundary" -> "ok"
7. Next try: Click on "Boundary". Then play with different settings of x(max), y(max) and z(max). For example, start taking them all to one. Then build-up your crystal by increasing for example x(max) to 2,3,4...
8. Point 6 to 8 can be repeated on graphite.
9. How are the two crystal structures different? Describe qualitatively.
10. What is the shortest distance between two atoms in diamond and graphite? Distances obtained using the most left positioned tool bar. Use the 5<sup>th</sup> tool from the top.

## VESTA Exercise sheet B

### Crystal structure of diamond and boron-nitride (cubic).

1. Download (and install) the soft-wave program VESTA from the web.  
<http://jp-minerals.org/vesta/en/download.html>
2. Find and download the diamond (C) and boron-nitride (BN) cubic VESTA files from:  
[http://www.misasa.okayama-u.ac.jp/~masami/pukiwiki/index.php?Vesta\\_data](http://www.misasa.okayama-u.ac.jp/~masami/pukiwiki/index.php?Vesta_data)
3. Open the downloaded files with VESTA.
4. Try the following on boron-nitride (cubic). Click on the "properties"-button -> "Single unit cell".
5. For clarity: click on "Edit" -> "Bonds" -> click on the row where the atoms are -> click on "Do not search atoms beyond the boundary" -> "ok"
6. Next try: Click on "Boundary". Then play with different settings of x(max), y(max) and z(max). For example, start taking them all to one. Then build-up your crystal by increasing for example x(max) to 2,3,4...
7. Point 4 to 6 can be repeated on graphite.
8. How are the two crystal structures different? Describe qualitatively.
9. What is the shortest distance between two atoms in diamond and boron-nitride? Distances obtained using the most left positioned tool bar. Use the 5<sup>th</sup> tool from the top.
10. What material properties do diamond and boron-nitride have in common. (Try google-up answers)

## VESTA Exercise sheet C

### Crystal structure of gold and iron.

1. Download (and install) the soft-wave program VESTA from the web.  
<http://jp-minerals.org/vesta/en/download.html>
2. Find and download the gold (Au) and iron (Fe) VESTA files from:  
[http://www.misasa.okayama-u.ac.jp/~masami/pukiwiki/index.php?Vesta\\_data](http://www.misasa.okayama-u.ac.jp/~masami/pukiwiki/index.php?Vesta_data)
3. Open the downloaded files with VESTA.
4. Try the following for gold: Click on the "properties"-button -> "Single unit cell".
5. For clarity: click on "Edit" -> "Bonds" -> click on the row where the atoms are -> click on "Do not search atoms beyond the boundary" -> "ok"
6. Next try: Click on "Boundary". Then play with different settings of x(max), y(max) and z(max). For example, start taking them all to one. Then build-up your crystal by increasing for example x(max) to 2,3,4...
7. Point 4 to 6 can be repeated on iron.
8. How are the structure of gold and iron different?
9. What is the shortest distance between two atoms for gold and iron? Distances obtained using the most left positioned tool bar. Use the 5<sup>th</sup> tool from the top.
10. If you google-up the mass of a gold and iron atoms, can you given this structure figure out the density (mass / volume) of both?

## VESTA Exercise sheet D

### Crystal structure of gold and table-salt (NaCl).

1. Download (and install) the soft-wave program VESTA from the web.  
<http://jp-minerals.org/vesta/en/download.html>
2. Find and download the VESTA files of gold (Au) and NaCl from:  
[http://www.misasa.okayama-u.ac.jp/~masami/pukiwiki/index.php?Vesta\\_data](http://www.misasa.okayama-u.ac.jp/~masami/pukiwiki/index.php?Vesta_data)
3. Open the downloaded files with VESTA.
4. Try the following for gold. Click on the "properties"-button -> "Single unit cell".
5. For clarity: click on "Edit" -> "Bonds" -> click on the row where the atoms are -> click on "Do not search atoms beyond the boundary" -> "ok"
6. Next try: Click on "Boundary". Then play with different settings of x(max), y(max) and z(max). For example, start taking them all to one. Then build-up your crystal by increasing for example x(max) to 2,3,4...
7. Point 4 to 6 can be repeated on NaCl.
8. How are the structure of gold and NaCl different?
9. Distances obtained using the most left positioned tool bar. Use the 5<sup>th</sup> tool from the top. What is heavier gold or table-salt? Why is that?

## **VESTA Exercise sheet E (Difficult)**

### **Crystal structure of gold, table-salt (NaCl), diamond and cubic zinc sulfide.**

1. Download (and install) the soft-wave program VESTA from the web.  
<http://jp-minerals.org/vesta/en/download.html>
2. Find and download the VESTA files of gold (Au), NaCl, diamond and cubic zinc-sulfide (ZnS) from:  
[http://www.misasa.okayama-u.ac.jp/~masami/pukiwiki/index.php?Vesta\\_data](http://www.misasa.okayama-u.ac.jp/~masami/pukiwiki/index.php?Vesta_data)
3. Open the downloaded files with VESTA.
4. Do these 4 materials have any structure in common?