

NIST

NIST Standard Reference Database 42

NIST Surface Structure Database (SSD) with Interactive Analysis and Visualization

Version 5.0

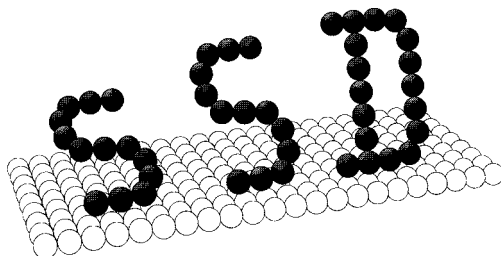
Installation and Quick Start

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PREFACE

The PC-based NIST Surface Structure Database (SSD) is aimed at scientists and students in physics, chemistry and materials sciences who wish to know and compare the detailed atomic-scale structures of surfaces obtained from experiment.

Version 5.0 of SSD is an improved 32-bit version of the software for use under Windows NT/2000/XP. Improvements have been made in the database manipulation and in the graphical visualization and analysis. Version 5.0 expands the database to nearly 1400 structure determinations and attempts to cover all known surface structures since the inception of surface crystallography in the early 1970s through the end of 2002.

The complete documentation for running SSD is available as on-line help within the program. This printed documentation provides information about hardware and software requirements and about software installation, as well as a guide to a quick start and easy use of the software. In addition, it provides illustrations of the 17 2-D space groups used to define surface structure symmetries.

The NIST Surface Structure Database can be obtained from NIST directly at the following address:

U.S. Department of Commerce
Standard Reference Data Program
National Institute of Standards and Technology
Building 820, Room 113
Gaithersburg, MD 20899

ACKNOWLEDGMENTS

We are grateful to the National Institute of Standards and Technology, particularly to the Standard Reference Data Program, for undertaking the support of SSD, as well as for providing professional advice and help in setting up and distributing this database. We are also much indebted to our consultants, Prof. J.B. Pendry and Prof. G.A. Somorjai, for helpful advice. We also thank the many authors who contributed their data through the SSDIN input program.

The work in Berkeley was supported in part by the Director, Office of Energy Research, Office of Basic Energy Sciences, Materials Sciences Division of the U.S. Department of Energy under Contract No. DE-ACO3-76SF00098.

Signed: P. R. Watson, Corvallis, Oregon
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April 2004

1. HARDWARE AND SOFTWARE REQUIREMENTS

The Surface Structure Database is designed to run on personal computers with the following hardware configuration:

- Intel® Pentium or compatible (AMD) processor;
- at least 64 MB of memory;
- (S)VGA graphics with at least 256 colors and color monitor with 800x600 pixels or higher resolution;
- 10 Mb of free hard disk space, 20 Mb for the installation;
- printer (optional; required for print output of listings, PostScript type for printing graphics).

The database has been tested on a variety of Intel® Pentium and similar systems from a number of manufacturers, but there is always the possibility of an incompatibility with some particular combination of hardware. If difficulties in installing or running SSD are encountered, please refer to the troubleshooting section or one of the authors, see Appendix C.

2. SOFTWARE INSTALLATION

The software is contained on a single CD-ROM as a single self-extracting INSTALL.EXE file. Before installation, check for the presence of a README.1ST file for any last-minute changes or additions that are not in this document.

When installing to a Windows system that allows users with different levels of rights, you will need to have administrator rights, or need to change your authorization and log on as administrator before you will be able to successfully install SSD 5.0.

Start the installation by either double-clicking on the file INSTALL.EXE on the CD via the Windows Explorer or My Computer, or by clicking on the Start button, selecting Run and entering the appropriate location for the installation file e.g. D:/INSTALL.EXE (if the CD-ROM drive is assigned the letter D:).

The installation process will prompt you several times to allow a choice of e.g. a particular directory for SSD 5.0 to reside, or whether to keep back-up copies of changed files. Many files necessary to the operation of Microsoft® Visual Basic as well as the database itself will be copied to your

computer. Depending upon the configuration of your particular computer and operating system, one or more restarts may be necessary.

The installation process also installs an Uninstall option, which allows you to remove SSD 5.0 from your system including many of the system files that had been installed.

Troubleshooting

You receive the error message **“SAO\DAO360 DLL could not be opened. Access denied.” Please check that your disk is not full and that you have access to the destination directory. Access denied.**

This error occurs when installing to a Windows system when logged on as a user that has no administrator rights. The solution is to change your authorization and log on as administrator and reinstall the program.

If you have other installation problems, please contact one of the authors listed in Appendix C.

3. QUICK START

The purpose of this section is to provide a quick way to obtain useful information from SSD. To that end, a simple generic session with SSD is presented, which you can follow step by step.

With this quick approach, access to all of the database information is gained, a graphical image of a structure of interest will be produced, and methods will be introduced to analyze the structure. Additional options will be found by simply opening the menus and trying the different options, or by following the links provided within the help text.

Further details are provided by accessing the **on-line help** at any time through the menu item Help, or by pressing the Help buttons provided in several windows, or by pointing near the appropriate window/entry field, pressing the left mouse button and then pressing the F1 key before releasing the mouse button.

Note that clicking on the left and right mouse buttons will here be called **L-clicking** and **R-clicking**, respectively. **D-clicking** means double-L-clicking (quickly left-clicking twice in succession).

Starting SSD

SSD is started like any other application under Windows 98/ME/2000/NT4/XP, e.g.:

- D-click on the SSD icon located on the desktop or in a program group on the desktop;
- or L-click on Start (on the bottom bar of Windows), then on Programs, and then on the SSD program name;
- or D-click on the file name `ssd5.exe` in the appropriate folder under Windows Explorer or under My Computer.

Browse Mode

Initially, SSD's title screen is displayed for a few seconds, followed by the SSD windows. SSD is now in its default "Browse Mode", and already displays data and a graph for the first structure in the database (by virtue of the alphabetical order of its "common name" shown in the top left box).

In this "Browse mode", all structures in the database can be accessed directly by scanning down the Structure List shown in the bottom right window. To select a different structure from the Structure List, first use the cursor keys or the vertical scrollbar at its right to find it. This is done by dragging the scroll button, L-clicking above or below it, or L-clicking on the arrows at top and bottom of that scroll bar, or by L-clicking on a structure in the list and then using the down-arrow, up-arrow, PageUp or PageDown keys to go down or up through the list. Alternatively you can type in the chemical symbol of the substrate and the cursor will jump to the first occurrence of that element. Then D-click on the small gray box to the left of the desired structure. This causes new data to be shown in the left "Summary window" and a new graph to be plotted in the graphics window at top right.

Search Mode

Suppose we wish to inspect the Rh(111)+c(4x2)-C₂H₃+CO structure (consisting of ethynidyne and carbon monoxide molecules coadsorbed on the Rh(111) surface). Browsing is not an efficient method to find it in the long Structure List. It is more effective to use SSD's "Search mode". To enter the Search mode, L-click on the **Search** button on the button bar near the bottom of the screen, or select the menu item Mode | Search. If you don't see the item Mode, you are looking at the "Graphics menu"; switch to the "Data menu" by L-clicking in a non-graphical window.

This opens a powerful Search criteria window, with which we can find structures through a variety of keywords or combinations of keywords. A brief description of the different options is shown in the window to the right of the Search Criteria window. We must now enter such search criteria into one or more boxes. The safest way to enter a criterion into a box is to open a "pick list" of available entries: L-click on the downward arrow at the right end of the box, scroll down to the desired entry, and L-click on that entry. It is also possible to directly type in keywords (including partial words).

Now enter 'Rh' into the Substrate box and 'CO' into the Adsorbate box (without the quotation marks). Then L-click on the **Search** button at bottom left of the Search criteria window. This causes the search to gather all applicable structures from the database into a "hit list". **Note** that by default a wildcard character (*) is added at the start and end of a criterion. In this case the result is that structures will be found that involve Rh alloys or compounds and/or adsorbates such as CO₂ as well as CO. This wildcard option can be turned off by removing the check mark labeled "Wildcards ON" below the criterion boxes. L-click on **Accept** to make these available in the Structure List window at the bottom right of the screen. **Note** also that SSD is not case-sensitive; it does not distinguish between CO and Co.

We could have been more selective, for example by also specifying a criterion for the Pattern (i.e. the particular LEED pattern of the structure), or some other aspect of the structure.

Whether we used the Browse mode or the Search mode, we should now select the desired Rh(111)+c(4x2)-C₂H₃+CO structure from the Structure list, by applying the procedure given above (scrolling as needed and then D-clicking on the gray box to the left of the desired structure).

Data Windows

We now discuss the variety of information that can be obtained about the last selected structure.

The left half of the screen is now occupied by the Summary window for the newly selected structure and gives general information about this structure. The **Help** button within this window provides further information about the type of data contained in this window. For example, if the meaning or purpose of some data box is unclear, an explanation is available using Help. (This same information is also available at any time through menu item Help.)

Additional data about this structure are available in other windows that can be reached by pressing one of the buttons at bottom left (or by selecting an item from the Windows menu list): **Expt/Th**, **2D cells**, **Coords**, or **Bonds**. Let's select the button **Expt/Th** or the menu item Experiment/Theory; a new window appears, showing a variety of details concerning the experimental and theoretical procedures that were used to obtain the data for this particular surface structure.

Explore the other data windows in the same way to view the 2-dimensional unit cells present in the structure, the coordinates of the different atoms, as well as selected bond lengths and angles.

Note that you can move the Data windows around and resize them, so as to see several windows simultaneously. To move a window, drag its title bar (i.e. point at its title bar, press and keep pressed the left mouse button, move the mouse pointer where desired and then let go the left mouse button). To resize a window, drag one of its borders or corners. You can later reset all the data windows at once to their original default positions and sizes by selecting Menu item Windows | Reset.

Graphics Window

The structural image in the top right window can be used to view the currently selected structure in a variety of ways. By L-clicking on its title bar, a new graphics menu (see graphics window of the Surface visualizer section) appears at top left above the data windows. This menu controls the graphics. (To return to the original "data menu", click on any data window or the Structure List.)

Note that you can move or resize the graphics window as described above for the other windows. You can also let it fill the screen by L-clicking on the middle button at top right (the "Maximize" button). To restore the graphics window to its default position and size, L-click in a non-graphics window, then choose menu item Windows | Reset.

The graphics window shows a piece of a surface (or interface) bounded by a rectangular box. By default you look down at an angle onto the surface, which is presented with perspective effect. Colors indicate chemical elements, as labeled at top left.

Changing views

The easiest change of the graphics is the view orientation; drag the mouse pointer (while keeping its left button pressed) to see the bounding box rotate around its vertical axis (azimuthal rotation about the surface normal) and around a horizontal axis (polar rotation). This is the default action of dragging the mouse, which is also achieved by dragging the mouse while keeping the **Alt** key pressed on the keyboard.

The size of the image can be changed by dragging the mouse pointer up or down the window while keeping the **Ctrl** key pressed on the keyboard.

The image can be shifted laterally and up or down by dragging the mouse pointer in the desired direction while keeping the **Shift** key pressed on the keyboard.

The degree of perspective effect can likewise be changed by dragging the mouse pointer up or down while keeping both the **Ctrl** and **Shift** keys pressed on the keyboard. Moving the mouse pointer all the way down gives parallel perspective. The parallel perspective and the default perspective can also be easily chosen through menu item View, then option Parallel projection or option Default perspective.

The image can also be rotated around the line of sight by dragging the mouse pointer up or down while keeping both the **Ctrl** and **Alt** keys pressed on the keyboard.

The default (drag = 3-dimensional rotation) can be changed via the menu item View | Drag; click on a different choice to modify the default action of dragging the mouse.

Other convenient actions include (see further below for procedures involved in some of these):

- set the view direction to be parallel to the x, y or z axes through menu item View, then View -> x, etc.
- set the "view focus" (that part of the surface which is centered on the screen) through menu item View | Set View Focus: then click on an atom which will be centered.

Some of the above actions require you to select specific atoms by pointing them out with the mouse. The line at the bottom of the graphics window tells you what to do in shorthand form. The first step is to L-click on the desired atom; it is sufficient to move the mouse pointer to any position on the visible part of that atom and then to L-click. Depending on the action that follows, you may have to select a second or additional atoms in the same manner, or R-click to start the requested action, or fill in a dialogue box.

Changing the presentation of the atoms

Several other changes of the graphical presentation are possible. These can be used for purposes of better viewing, for showing bonding relationships, or for embellishing the view. The latter is particularly useful in order to prepare and export a publication-quality plot. All these changes are found as different options accessed through menu item Settings.

First, let's change the type of ball that represents an atom. First make sure that the graphics menu is displayed above the data windows (if not, L-click on the graphics window to activate it and its menu). Then select menu item Settings | Atom Design. Now choose the type of atom display desired, e.g. brilliant balls. **Note** that plotting these "brilliant balls" takes more time than the original "plain balls (one color)". So one would normally first plot with a plainer design to adjust the many variables that go into a pleasing figure, before doing the final plotting, especially when the plot involves many atoms.

Other options include:

- change the drawn atomic radii collectively either by scaling ("relative" change) or one element at a time in Angstrom ("absolute" change), through menu item Settings | Atom radii.
- hide and revive atoms, i.e. make them temporarily invisible, through menu item Settings | Atom hide/revive.
- change drawn bonds, through menu item Settings | Atom bonds.
- change the bounding box dimensions to allow more or fewer atoms to be seen, through menu item Settings | Surface section.

Explore the Settings menu to find other ways to change the plot.

Analysis

Another powerful set of options is provided to "analyze" the structure; they allow you to measure a variety of quantities in the current structure, such as

bond lengths (in Angstroms), bond angles (in degrees), and interlayer distances (in Angstroms). See the menu item Analysis for the various options that are available.

As an example, let us find the bond length between two atoms. Again, make sure that the graphics menu is displayed above the data windows (if not, L-click on the graphics window to activate it and its menu). Choose menu item Analysis, then option Atom distances/vectors. At the bottom of the graphics window now appears the instruction

"Atom distance/vector AB: L-click 2 diff. atoms A,B; R-click evaluates".

This tells you to first L-click on the two atoms in question (if they are hidden behind other atoms, you may have to exit the analysis (R-click) and rotate the view). See above on how to L-click on an atom. After each atom has been selected, you will see its identity, coordinates and radius displayed. After selecting the second atom, R-click. This results in a display of the interatomic distance (and, for comparison, the sum of the current atomic radii as SumRad between parentheses), followed by the vector pointing from the first to the second atom, all in Angstroms. The vector is also drawn as a white line on the plot

Note that you cannot select (point at) an invisible atom. On the other hand, you may on purpose make atoms invisible so as to reveal deeper-lying atoms and analyze them. This feature becomes most useful in inspecting very complex surface structures.

Compare Mode

It is often desirable to compare visually different structures, or to compare visually the same structure as determined in different studies. This is possible by switching SSD to its "Compare mode". In that mode up to 3 different structures can be drawn in separate windows and individually displayed for optimum comparison.

Let's compare some structures of O on Ni(100). To narrow down the list from which to select, we first do a **Search**, by specifying 'Ni' for the Substrate, '100' for the Substrate Face, and 'O' for the Adsorbate. L-click **Search**, then **Accept**, resulting in a shorter hit list being displayed in the Structure list. Next we must choose one structure from the Structure list, e.g. the first Ni(100)+c(2x2)-O that occurs.

Now L-click the **Compare** button on the button bar near the bottom of the screen. A "Compare structures" window is opened, which allows you to select 1 or 2 other structures for comparison.

We can select a second structure from the same hit list by leaving the "Select from Search" option active. Let's select the last Ni(100)+c(2x2)-O in the list, by D-clicking on the gray box in front of its name, or by highlighting the entry and clicking on the Select button. (It is also possible to select structures from the complete database by setting "Select from Database".)

This results in a second graphics window being opened, displaying the second structure. Also, this second structure is listed as "Comparison 1" in the Compare structures window.

To select a third structure for comparison, first activate the button to the right of the "Comparison 2" line in the Compare structures window. Then select another structure from the Structure List.

Remember that you can move and resize the windows to obtain the most effective display. And within each window, you can adjust all graphical features as discussed above.

You can close any graphics window by L-clicking on its X button (at top right of each window), or by selecting its menu item File | Exit.

You can also replace any of the comparison structures by activating the button to its right in the Compare Structures window and selecting another structure.

L-Click on **Cancel** to quit the comparisons and close any excess graphical windows.

Termination of SSD

SSD is terminated by any of the standard Windows methods, such as:

- select menu item File, option Exit.
- or L-click on the X button in the top right corner of the screen.

Appendix A

THE 17 TWO-DIMENSIONAL SPACE GROUPS

This Appendix illustrates the 17 two-dimensional space groups that exist for surfaces and interfaces in strictly two dimensions. SSD characterizes both the ideal substrate terminations and the actual surfaces by their respective space groups.

Additional space groups are possible if one allows symmetry operations across the interface, e.g., mirror symmetry about the interface, as may happen in twinning of two crystals. Then 80 space groups exist; they have been tabulated by Wood (1964). However, situations where any of these additional space groups might be useful are rare in surface science. The 17 two-dimensional space groups always remain applicable, even if they do not convey all the useful information in those rare cases.

The following diagrams show, for each of the 17 two-dimensional space groups:

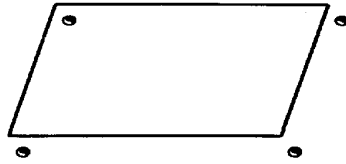
- one unit cell outlined in heavy lines (where not overdrawn by thin symmetry lines);

- all applicable symmetry elements: 2-, 3-, 4- and 6-fold rotation axes (perpendicular to the surface), drawn as black ovals, triangles, squares and hexagons, respectively; mirror lines (planes perpendicular to the surface) drawn as thin lines, glide lines (planes perpendicular to the surface) as dashed lines;

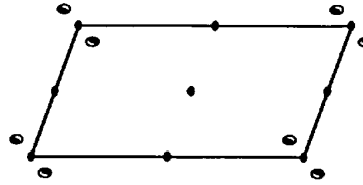
- a general point in the unit cell, symbolized by a yin-and-yang figure, together with all other points equivalent to it by symmetry; the left-handed and right-handed yin-and-yang symbols show how orientations are mirrored and rotated into each other.

The 17 two-dimensional space groups

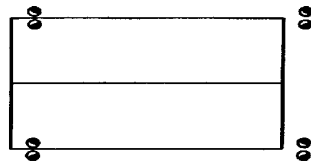
1. p1 - oblique



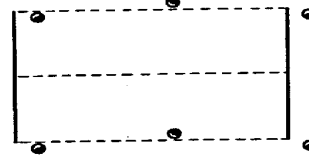
2. p2 - oblique



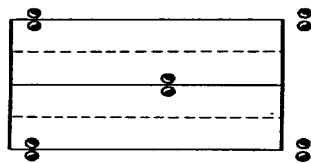
3. pm - rectangular



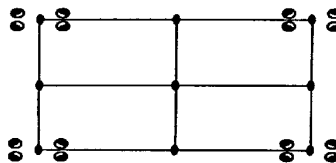
4. pg - rectangular



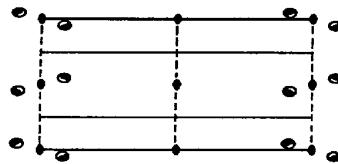
5. cm - rectangular



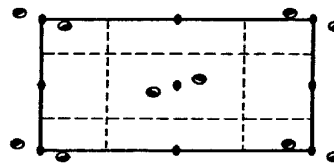
6. pmm - rectangular



7. pmg - rectangular

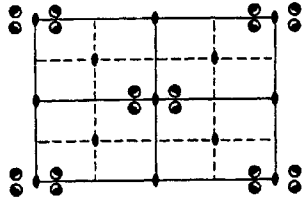


8. pgg - rectangular

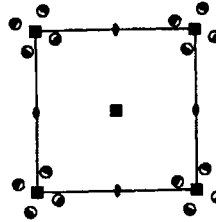


The 17 two-dimensional space groups - *continued*

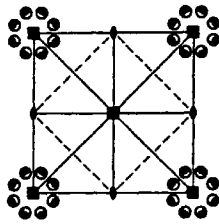
9. cmm - rectangular



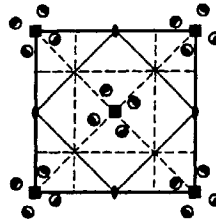
10. $p4$ - square



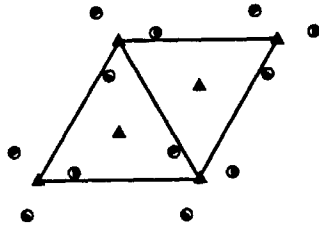
11. $p4m$ - square



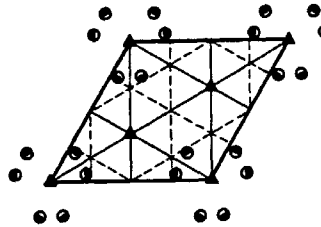
12. $p4g$ - square



13. $p3$ - hexagonal

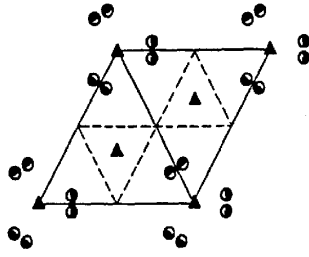


14. $p3m1$ - hexagonal

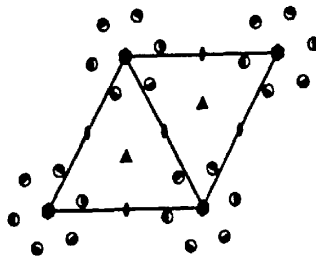


The 17 two-dimensional space groups - *continued*

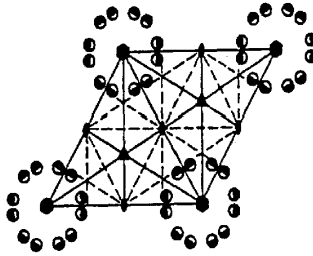
15. p31m - hexagonal



16. p6 - hexagonal



17. p6m - hexagonal

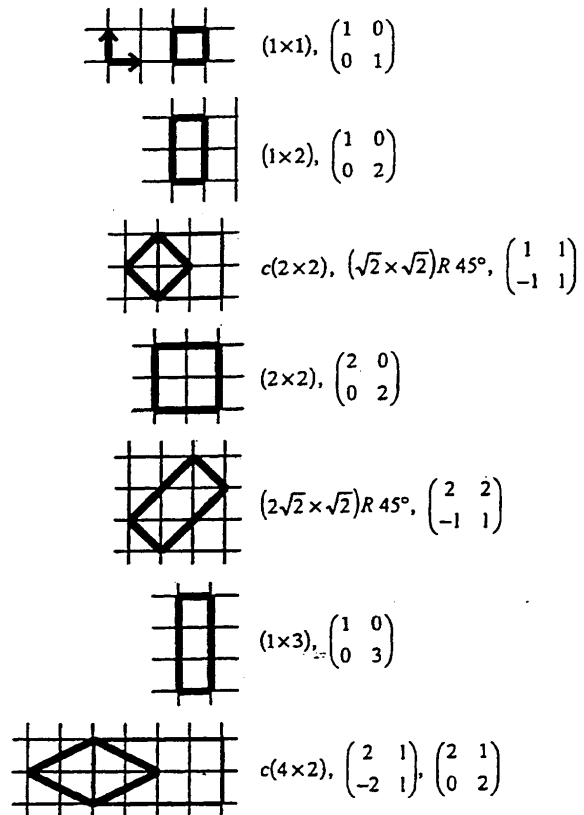


Appendix B

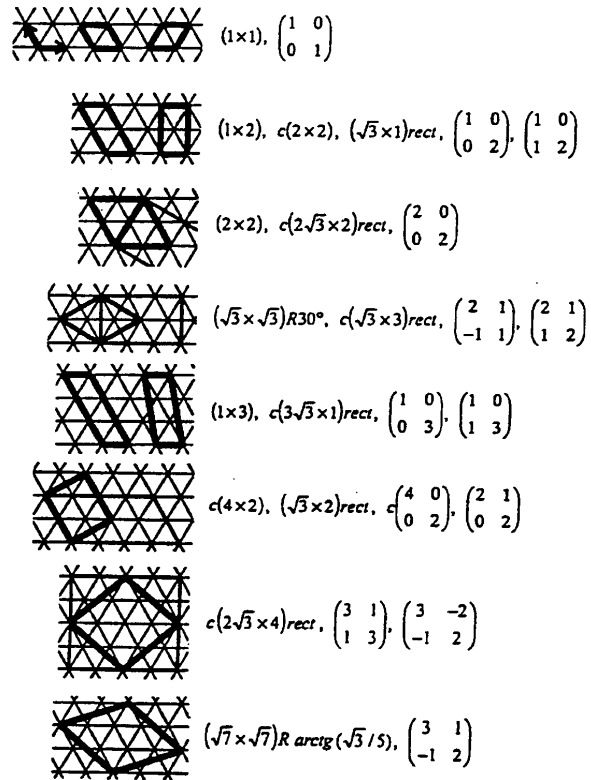
EXAMPLES OF SUPERLATTICE CELLS

This Appendix illustrates two-dimensional unit cells and their notations.

Superlattices on square substrate lattices



Superlattices on hexagonal substrate lattices



Appendix C

CONTACTS

If you have questions or comments about the database, the Standard Reference Data Program would like to hear from you. Please contact:

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