

## Semper 6 Command Reference

### base

<b>keys:</b>	<b>[from]</b>	<code>&lt;number&gt;</code>	<i>Plist</i> picture
	<b>[to]</b>	<code>&lt;number&gt;</code>	output picture
	<b>position</b>	<code>&lt;x&gt;, &lt;y&gt;</code>	centre of region to which fit is restricted
	<b>radius</b>	<code>&lt;number&gt;</code>	radius of region to which fit is restricted
	<b>numbers</b>	<code>&lt;n1&gt;, &lt;n2&gt;</code>	serial number of positions to which fit is restricted
	<b>tolerance</b>	<code>&lt;number&gt;</code>	fractional deviation from initial (estimated) lattice sites beyond which sites are excluded from fit
	<b>mark</b>	<code>&lt;number&gt;</code> <code>&lt;yes or no&gt;</code>	mark the final deviations of all positions from the lattice on the display
	<b>times</b>	<code>&lt;number&gt;</code>	if <i>mark</i> , magnification of display marking
<b>options:</b>	<b>uvonly</b>		fit lattice base vectors $u$ , $u2$ and $v$ , $v2$ only, preserving lattice origin $w$ , $w2$
	<b>verify</b>		verify details of fitting process at the console

Use the **base** command to fit a lattice to a list of positions in a *Plist* picture. This command refines initial estimates that you provide of the lattice base vectors  $u$  and  $v$  and the lattice origin  $w$ , using a least-squares criterion and reports the quality of the resulting fit. For further detail of *Plist* pictures, refer to *Appendix A: Picture Types*.

Note that the commands **peaks** and **xwires list** produce a list of positions that can be used by **base** to fit a lattice.

### Examples

```
u=10,0 v=0,10 w=0,0; base 51
```

This command fits a lattice, roughly 10 pixels square, to sites listed in picture 51.

```
base 51 radius 100 position w,w2 mark display
```

This command fits positions within 100 pixels of the lattice origin  $w$ , and marks the final deviations on the display.

```
base numbers 100,150 uvonly verify
```

This command fits positions 100 to 150 only, with the lattice origin fixed at the picture origin, printing

**base**

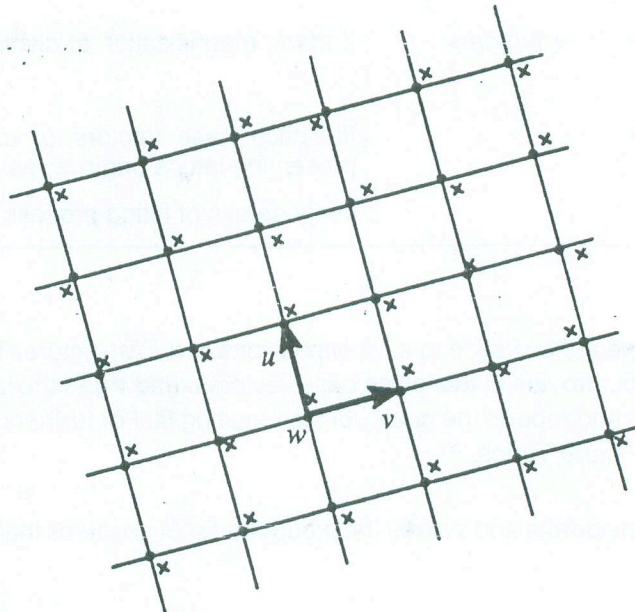
details of the fitting process at the console.

```
base 51 to 52 tolerance .1
```

This command produces a new *Plist 52* containing only those positions from 51 that lie within 0.1 lattice vectors of a fitted lattice site.

**Description**

**base** refines the values that you supply for the base vectors  $u$  and  $v$  and the lattice origin  $w$ . If you can supply an accurate value for the lattice origin,  $w$ , (for example, because you are fitting a power spectrum for which  $w$  must be 0,0), you can suppress the fitting of  $w$  using the **uonly** option. The diagram below illustrates the **base** command.



$w$  = lattice origin

$u, v$  = lattice base vectors

$\times$  marks position originally supplied in *Plist* picture

The initial estimates that you provide of  $u$ ,  $v$  and  $w$  (in picture coordinates) should be accurate enough to permit correct indexing of most positions. If you cannot achieve such accuracy, restrict the fit initially to a limited region and then use **base** a second time without the restriction. To restrict a fit to a region use one of the keys: **position** and **radius**.

To prevent a few spurious positions from biasing the fitted lattice, positions are ignored if they are not reasonably near a site of the estimated lattice – specifically, if their indices (coordinates in terms of the lattice base vectors) are not within 0.3 of an integer. The key **tolerance** allows you to alter this threshold value; a value of 0.5 or greater eliminates selection on this basis.

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If you specify the key **to** explicitly, as in the last command example, an output *Plist* is produced which includes only those positions included in the fitting process (that is, those within any defined subregion and within the relevant tolerance of the lattice).

**base** sets the variables *n* and *r* to the number of positions fitted, and their *r.m.s.* deviation respectively. If **mark** is set, the final deviations of all positions from the lattice are marked via small lines drawn from the positions in the directions of the corresponding lattice site, but 5 times larger than the actual deviation for visibility. You can alter the magnification factor of these marking lines using the **times** key.

#### Notes

restrictions:	<i>Plist</i> type pictures only
display marking:	final position deviations
form used internally:	complex
variables used:	<i>u</i> (2), <i>v</i> (2) (initial estimates for lattice base vectors) <i>w</i> (2) (initial estimate for lattice origin)
variables set:	<i>u</i> (2), <i>v</i> (2) (base vectors of fitted lattice) <i>w</i> (2) (origin of fitted lattice) <i>n</i> (number of sites included in fit) <i>r</i> (r.m.s deviation in source pixels between included sites and final fitted lattice)
see also:	<b>lattice, peaks, strain, xwires list</b>

#### Defaults and Ranges

keys/options	defaults	range
<b>[from]</b>	current picture number, held in the variable <i>select</i>	valid picture number
<b>[to]</b>	no output	valid picture number
<b>position</b>	position 0,0	within bounds of picture (real numbers)
<b>radius</b>	infinite	real number
<b>numbers</b>	all positions	1 to total number of points in the <i>Plist</i> picture
<b>tolerance</b>	tolerance 0.3	real number in range 0 to 0.5
<b>mark</b>	mark off	see <i>Appendix C</i>
<b>times</b>	times 5	positive integer
<b>verify</b>	verification off	