

## strain

<b>keys:</b>	<b>[from]</b>	<number>	source picture
	<b>[to]</b>	<number>	output picture
	<b>tolerance</b>	<number>	fractional deviation from initial (estimated) lattice sites, beyond which sites are excluded from fit
	<b>times</b>	<number>	if <b>mark</b> , magnification of display marking
	<b>mark</b>	<number> <yes> or <no>	mark deviations from lattice on display
<b>options:</b>	<b>verify</b>		list details of fitting process at console

Use **strain** to deduce local strain levels for distorted crystals from a list of unit cell positions, and re-sort the list into ascending strain order.

## Examples

```
u=10,0 v=0,10 w=0,0; strain 50 to 91
```

This command refines the lattice parameters  $u, v, w$  so as to fit the positions that are listed in picture 50. It outputs a revised list of positions, sorted in order of increasing strain level, to 91.

```
strain 999 tolerance 0.2 verify
```

This command re-sorts picture 999 by local strain level, excluding any positions with a fractional deviation from the nearest lattice site that exceeds 0.2. Information about the command process is sent to the console.

## Description

Note that in the initial stages of processing (the lattice fitting) **strain** works in the same way as **base**, although it has fewer options.

**strain** also evaluates a local strain measure for each position having at least two neighbours (defined as other listed positions for which the lattice coordinates differ from those at the first by values within **tolerance** of unity). The local strain measure is the *r.m.s.* fractional displacement difference between the position itself and each of its neighbours. **strain** stores the strain values in the list instead of the original height or mass values, if these are present, and resorts the list, omitting positions for which the strain cannot be estimated. You can then use the **motlf** command to make averages on the basis of selected strain levels only.

## Semper 6 Command Reference

### strain

If you specify a display using the **mark** key, **strain** marks all deviations from the lattice on the display. See *Appendix C, Semper Keys and Options* for details of the **mark** key. Use the **times** key to specify the magnification factor for the display marking.

#### Notes

variables used:	$u, u2, v, v2$ (initial estimates for lattice base vectors) $w, w2$ (initial estimate for lattice origin)
variables set:	$u, u2, v, v2$ (base vectors of fitted lattice) $w, w2$ (origin of fitted lattice) $n$ (number of sites included in fit) $r$ (r.m.s. deviation in source pixels between included sites and final fitted lattice)
see also:	<b>base, motif</b>

#### Defaults and Ranges

keys/options	defaults	range
[from]	current picture, held in the variable <i>select</i>	valid picture number
[to]	source picture	valid picture number
tolerance	tolerance 0.3	real number
times	times 5	positive integer
mark	mark off	see <i>Appendix C</i>
verify	verification off	