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Supporting information for article:

Epitaxies of Ca-sulfates on calcite (CaCO₃). II. The main {010}, {001} and {100} forms of bassanite (CaSO₄·0.5H₂O) epi-deposited on the substrate form of {10.4} calcite

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Calcite is made by three supercells; each of them has multiplicity ($2\times$) and is described by vectors and angles comprised between them, and that is: i) $[020] = 9.979$, $\frac{1}{3}\times[\bar{4}11] = 9.516$, $\delta = 121.62^\circ$; ii) $-\frac{1}{3}\times[45\bar{1}] = 9.516$, $-[020] = 9.979$, $\delta = 121.62^\circ$, and $-\frac{1}{3}\times[\bar{4}11] = 9.516$, $\frac{1}{3}\times[45\bar{1}] = 9.516$, $\rho = 116.75^\circ$. The pseudo-hexagonal supercell with multiplicity ($6\times$), occupies an area of 242.58 \AA^2 . The rectangular 2D-cell on the (10.4) face is drawn in Figure S1 (upper left side), while an example of one 2D-supercell has been drawn as well in the same figure (lower left side).



Figure S1. The pseudo-hexagonality of the cleaved $\{10.4\}$ form of calcite. A ($6\times$) supercell, (right side), made by three ($2\times$) supercells, (left, lower side) is shown. The smallest 2D-cell of $\{10.4\}$ is also drawn (upper left).

Table S1. Other 2D-LC between $\{001\}_{\text{Bss}}$ and $\{10.4\}_{\text{Cc}}$.

Ranking	$\{10.4\}_{\text{Cc}}$ lattice vectors (\AA)	$\{001\}_{\text{Bss}}$ lattice vectors (\AA)	Max. linear and area misfit ($\Delta\%$)	Obliquity ($^\circ$)	Notes
case (2c)	$\frac{1}{3}[\bar{4}41] = 12.8546$ $[43\bar{1}] = 24.816$	$[100] = 12.032$ $[\bar{1}30] = 24.013$	-6.95 -3.34		No twin axis
2D cell area (\AA^2) and multiplicity	283.033 ($7\times$)	249.87 ($3\times$)	-13.27	0	Coherent linear misfits
case (4a)	$[42\bar{1}] = 24.309$ $3[010] = 14.969$	$2[100] = 24.064$ $2[010] = 13.86$	-1.02 -8.00		$[010]_{\text{Bss}}$ twin axis
2D cell area (\AA^2) and multiplicity	363.901 ($9\times$)	333.166 ($4\times$)	-9.22	0	Coherent linear misfits
case (4b)	$\frac{2}{3}[\bar{4}11] = 19.032$ $5[010] = 24.948$	$[1\bar{2}0] = 18.349$ $[210] = 25.017$	-3.72 +0.276		$[210]_{\text{Bss}}$ twin axis
2D cell area (\AA^2) and multiplicity	404.334 ($10\times$)	416.458 ($5\times$)	+2.99	6.71	Opposite linear misfits