

# Heteroepitaxial Growth of Gold on Silicon by Galvanic Displacement

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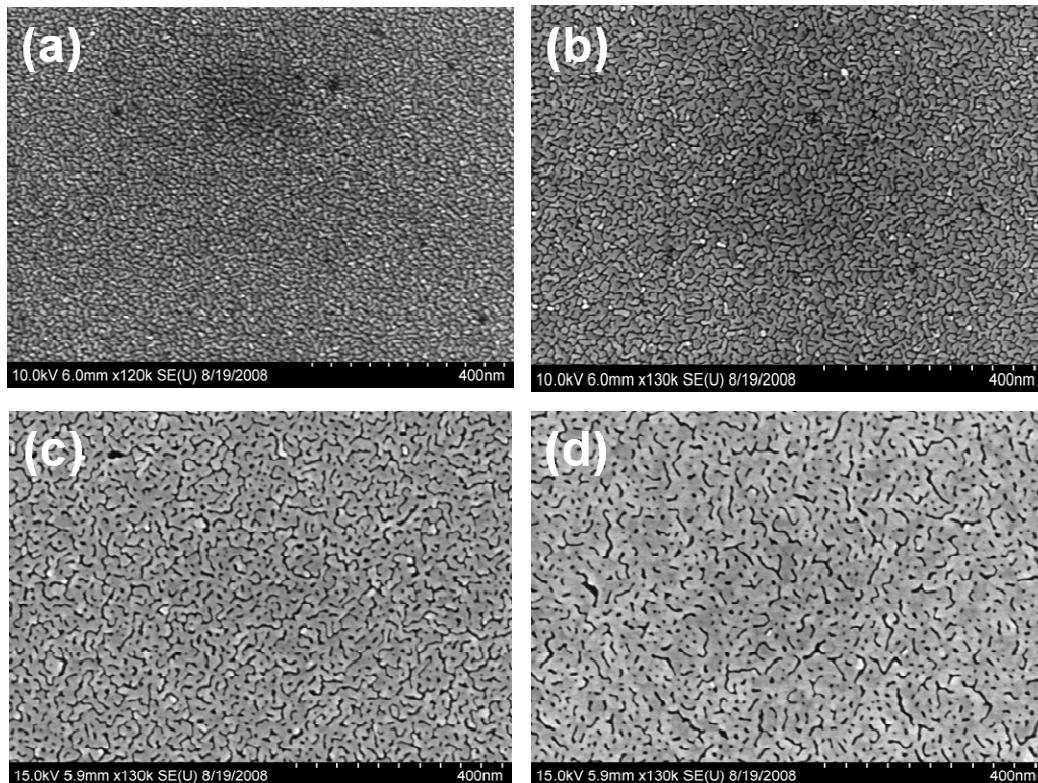


Figure S1. Scanning electron micrographs for Au galvanically displaced on Si(111) after immersing the silicon substrate in 0.1 mM  $\text{KAuCl}_4$  (aq) and 1% HF (aq) for different immersion times. (a) 2.5 min; (b) 5 min; (c) 7.5 min; (d) 10 min.

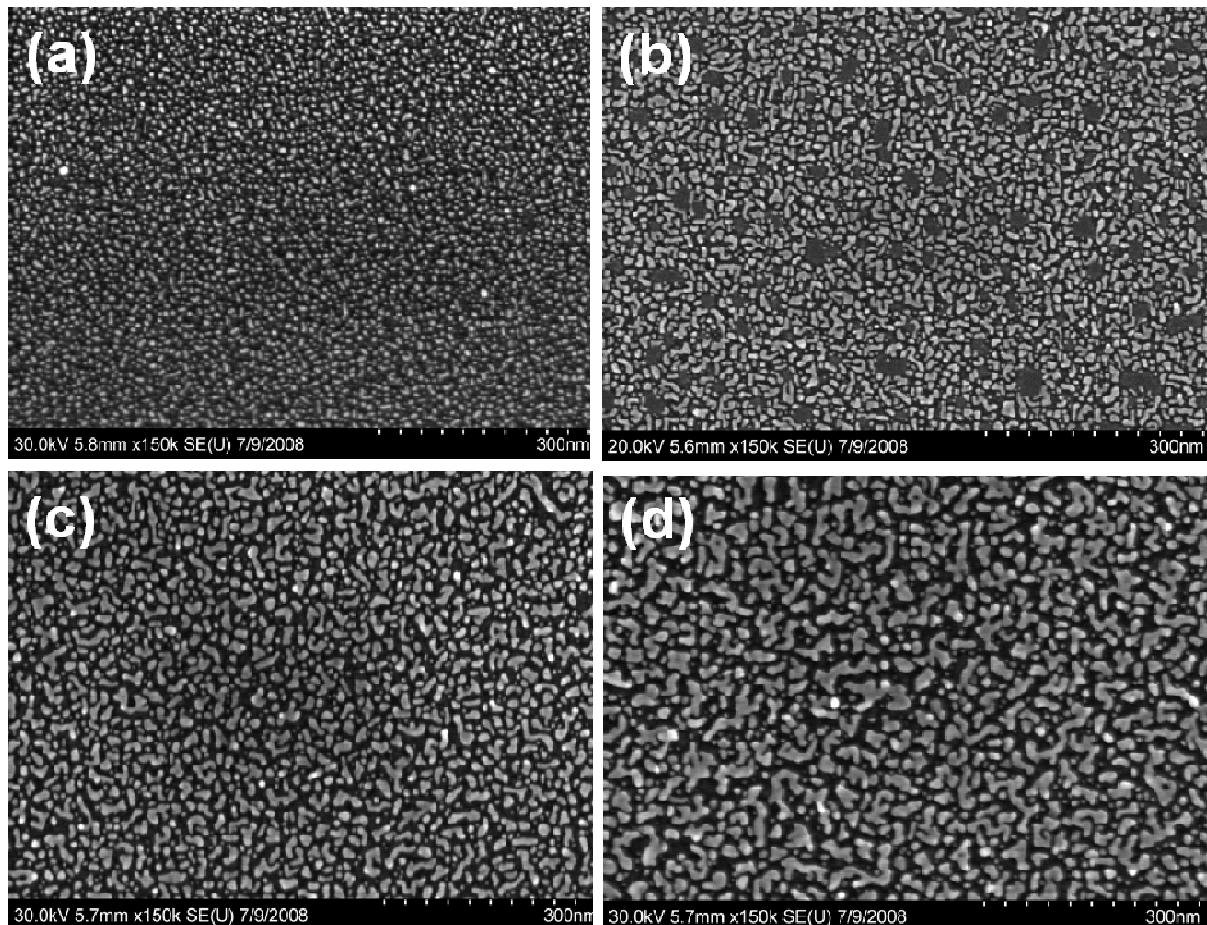


Figure S2. Scanning electron micrographs for Au galvanically displaced on Si(100) after immersing the silicon substrate in (0.1 mM KAuCl<sub>4</sub> (aq) and 1% HF (aq)) for different immersion time. (a) 2.5 min. (b) 5 min. (c) 7.5 min. (d) 10 min.

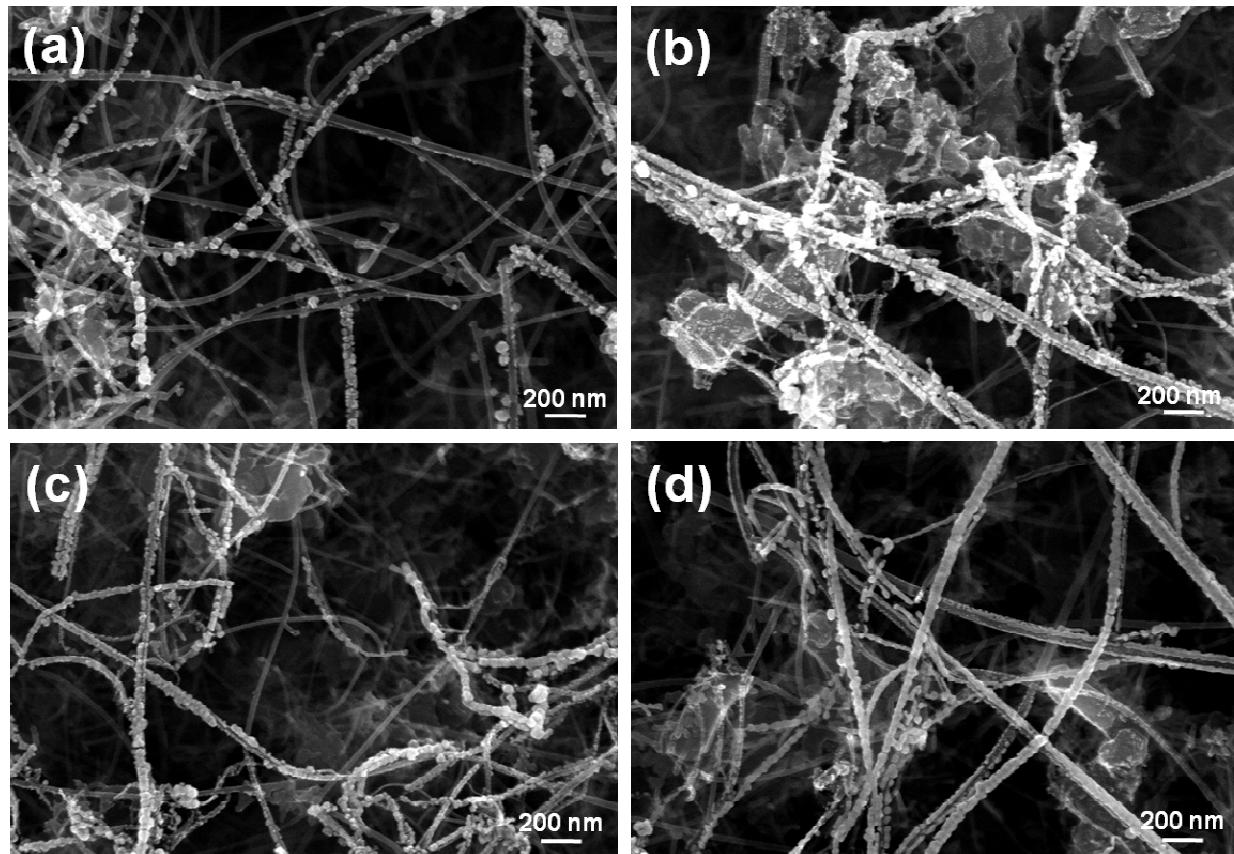


Figure S3. Scanning electron micrographs for Au galvanically displaced on Si NWs with 1 mM  $\text{KAuCl}_4$  (aq) and 1% HF (aq) for different exposure times. (a) 30 s; (b) 60 s; (c) 90 s; (d) 120 s.

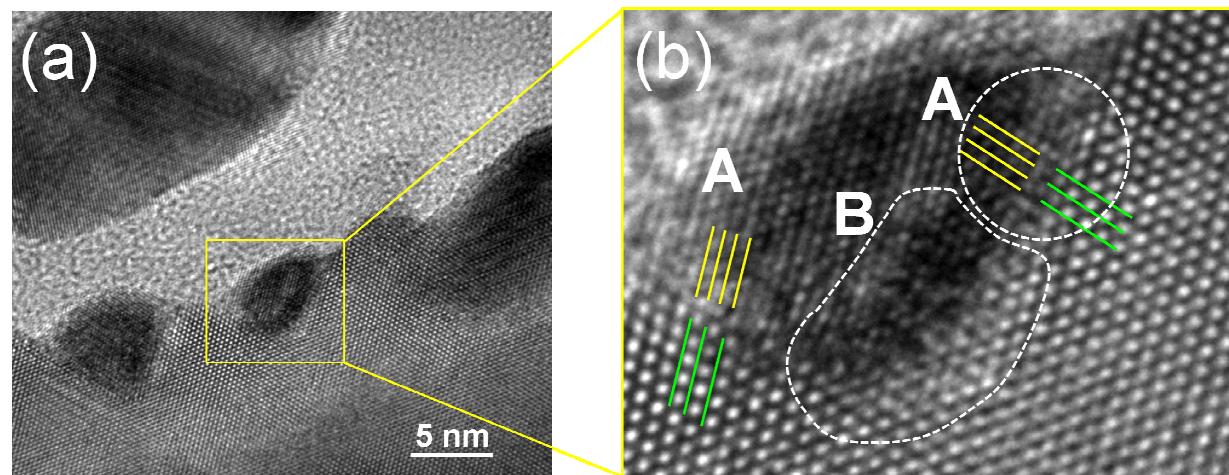


Figure S4. (a) Cross-sectional HRTEM images for Au-Si(100) interface formed by immersion in 0.1 mM  $\text{KAuCl}_4$  (aq) and 1% HF (aq) for 7.5 min. (b) HRTEM image, of the selected area in image (a), showing different areas marked A and B. Areas A and B show some areas have a very clear coincident gold and silicon lattices, whereas others appear less ordered, respectively.

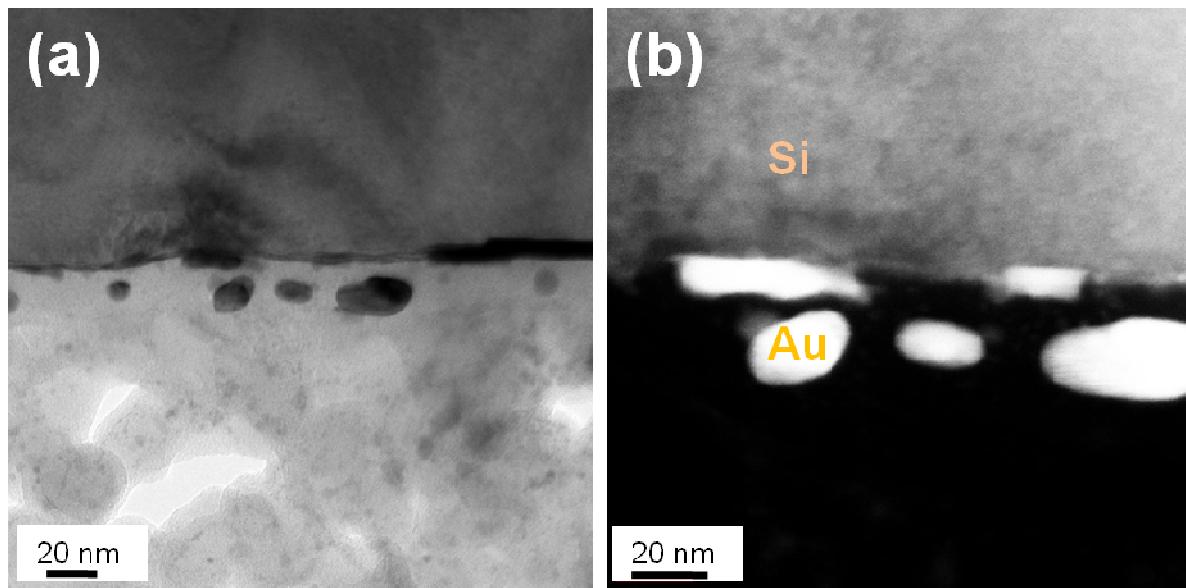


Figure S5. Cross-section transmission electron microscopy (TEM) images for Au galvanically displaced on Si(111) after immersing the silicon substrate in 0.1 mM KAuCl<sub>4</sub> (aq) and 1% HF (aq) for 7.5 min. (a) Bright field TEM image. (b) High-angle dark-field image.

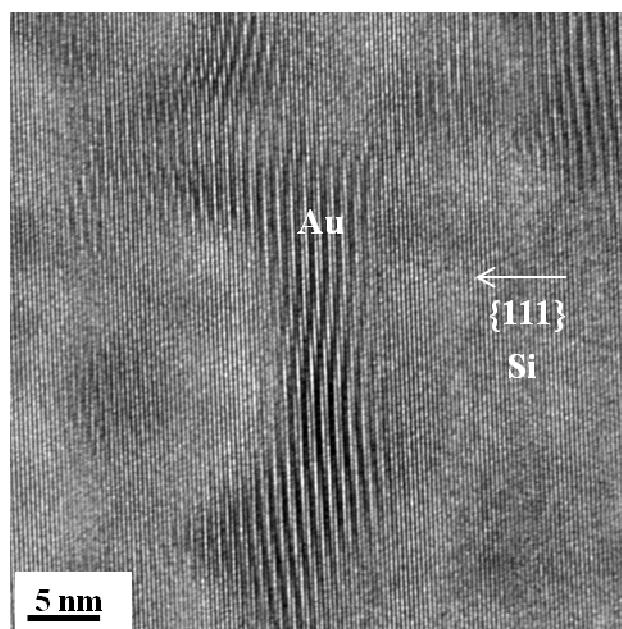


Figure S6. HRTEM image for gold on Si(111), formed by immersing the silicon substrate in 0.1 mM KAuCl<sub>4</sub> (aq) and 1% HF (aq) for 1.5 min. The image was taken close to the [1̄23] zone axis.

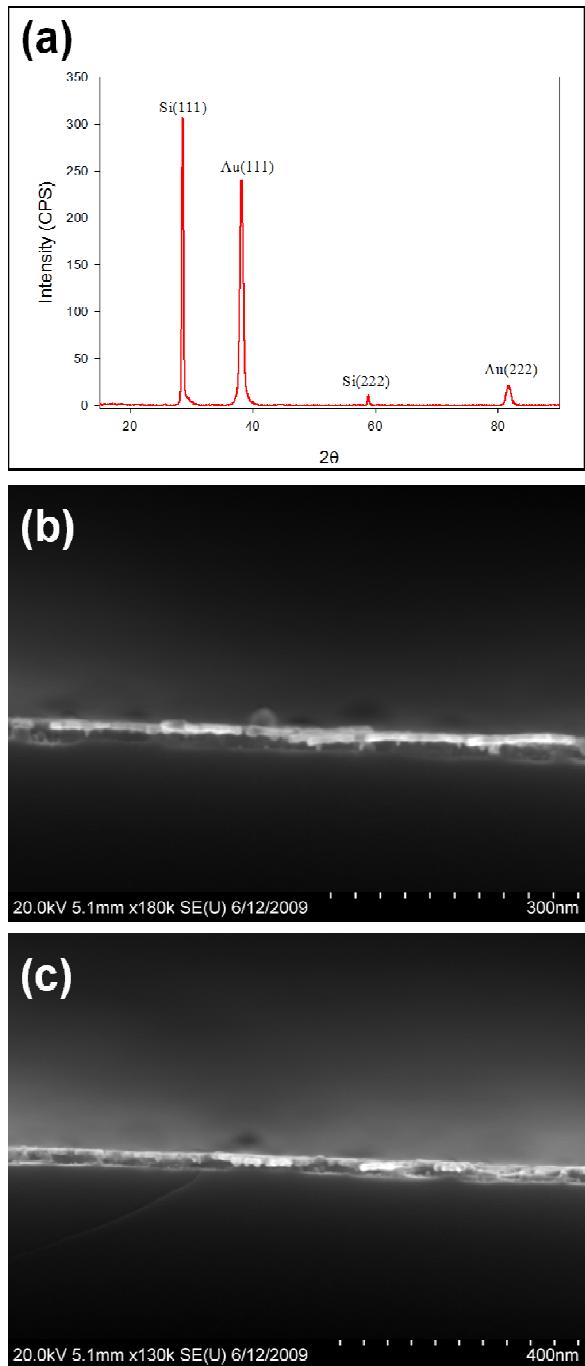


Figure S7. (a) X-ray diffraction (XRD) for Si(111) after immersion in 0.1 mM  $\text{KAuCl}_4$  (aq) and 1% HF (aq) for 20 min. The XRD spectrum indicates the preferential orientation of gold for the (111) plane and supports epitaxial growth of gold on Si(111). (b) and (c) are cross sectional SEM images for Au-Si sample from which the XRD (a) was observed.

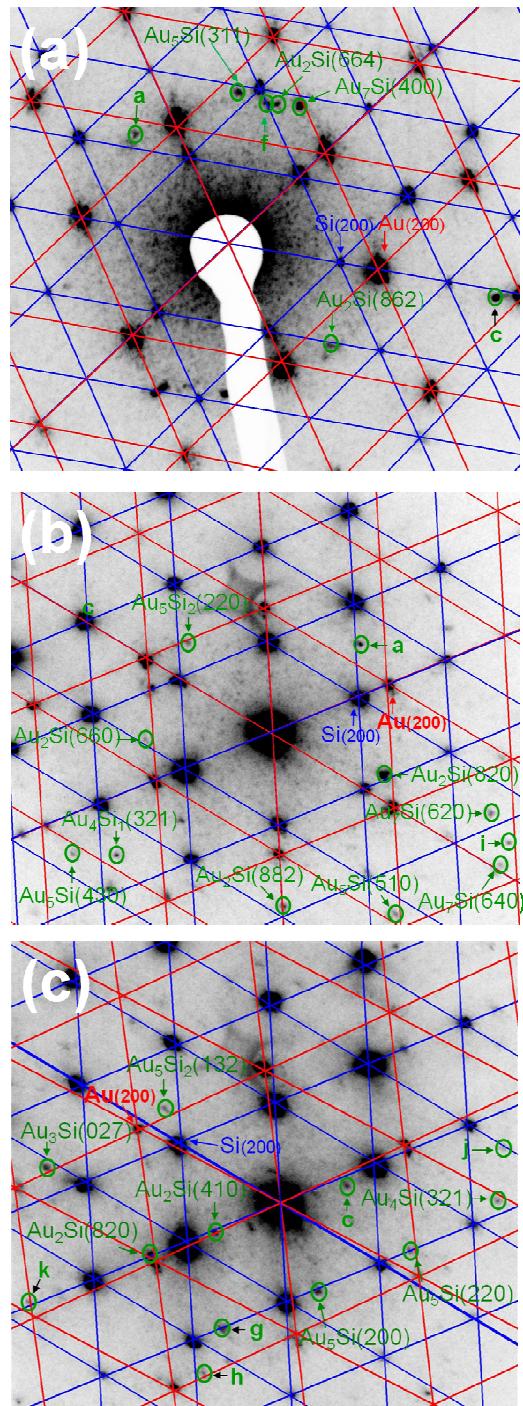


Figure S8. Indexed nanobeam diffraction patterns taken using a nanoprobe of about 20 nm in diameter of cross-sectional Au-Si samples prepared by immersion of the silicon substrate in 0.1 mM KAuCl<sub>4</sub> (aq) and 1% HF (aq) for 7.5 min. All images were taken close to the (110) zone axis. (a) The Au/Si(111) interface. (b) and (c) from Au/Si(100) interfaces at different locations. Blue and red lines are for silicon and gold planes, respectively.

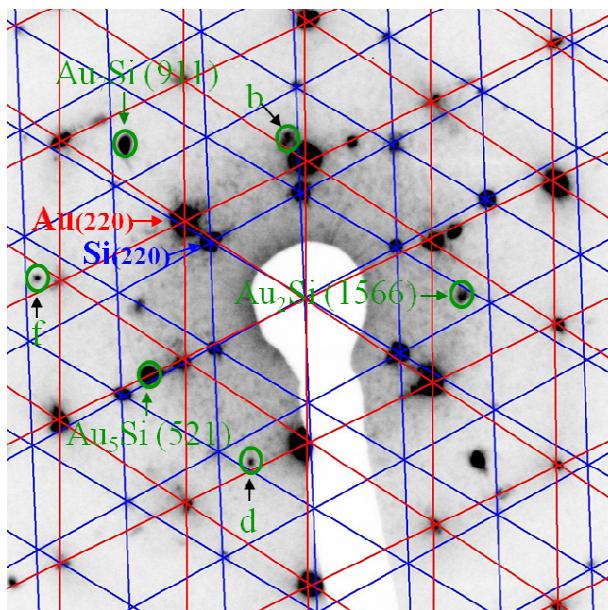


Figure S9. Nanobeam diffraction pattern taken close to the [111] zone axis of an area on a Si nanowire with a single gold nanoparticle with planes for gold silicides indicated.

planes	d measured, Å	silicides	d expected, Å
Si(111)	Standard		3.13
Si(200)	2.72		2.71
Au(111)	2.33		2.36
Au(200)	2.04		2.04
a	2.10	----	
b	2.17	Au <sub>2</sub> Si(862)	2.17
c	1.13	----	
d	1.96	Au <sub>7</sub> Si(400)	1.96
e	2.08	Au <sub>2</sub> Si(664)	2.10
f	2.12	----	
g	2.04	Au <sub>5</sub> Si(311)	2.03

Table 1a. Analysis of the nanobeam diffraction pattern (text, Figure 5a).

planes	d measured, Å <sup>o</sup>	silicides	d expected, Å <sup>o</sup>
Si (111)	standard		3.13
Si (200)	2.71		2.71
Au (111)	2.36		2.36
Au (200)	2.02		2.04
a	2.33	----	----
b	2.36	Au <sub>2</sub> Si(820)	2.36
c	2.32	Au <sub>2</sub> Si(660)	2.30
d	2.34	Au <sub>5</sub> Si <sub>2</sub> (220)	2.34
e	1.49	Au <sub>4</sub> Si(321)	1.49
f	1.70	Au <sub>2</sub> Si(882)	1.70
g	1.34	Au <sub>5</sub> Si(430)	1.35
h	1.25	Au <sub>7</sub> Si(620)	1.24
i	1.12	----	----
j	1.33	Au <sub>5</sub> Si(510)	1.33
k	1.11	Au <sub>7</sub> Si(640)	1.09

Table 1b. Analysis of the nanobeam diffraction pattern (text Figure 5b).

planes	d measured, Å	silicides	d expected, Å
Si (111)	standard		3.13
Si (200)	2.71		2.71
Au (111)	2.33		2.36
Au (200)	2.02		2.04
a	4.63	Au <sub>2</sub> Si(410)	4.72
b	2.34	Au <sub>2</sub> Si(820)	2.36
c	4.63	----	----
d	3.45	Au <sub>5</sub> Si(200)	3.37
e	2.34	Au <sub>5</sub> Si(220)	2.38
f	2.17	Au <sub>5</sub> Si <sub>2</sub> (132)	2.16
g	2.34	----	----
h	1.76	----	----
i	1.48	Au <sub>4</sub> Si(321)	1.48
j	1.39	----	----
k	1.19	----	----
l	1.37	Au <sub>3</sub> Si(027)	1.38

Table 1c. Analysis of the nanobeam diffraction pattern (text Figure 5c).

planes	d measured, Å <sup>o</sup>	silicides	d expected, Å <sup>o</sup>
Si(220)	standard		---
Au(220)	1.44		1.44
a	1.27	Au <sub>2</sub> Si(1566)	1.28
b	1.27	----	----
c	1.22	Au <sub>5</sub> Si(521)	1.23
d	1.22	----	----
e	0.87	Au <sub>7</sub> Si(911)	0.86
f	0.74	----	----

Table 1d. Analysis of the nanobeam diffraction pattern (text Figure 5d).