Supporting Information to

Interaction of chiral L-dialanine with Cu(100)

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S1. Stability of dialanine as a function of temperature

Our experiments are carried out by evaporating L-dialanine power from a heated crucible. It is important to ascertain that L-dialanine is evaporated as such and that it does not crack or decompose at temperatures at which evaporations are performed. To check the stability of L-dialanine, a thermogravimetric test (TGA) was carried out,[1] in which the loss of mass of dialanine in a crucible was measured as a function of temperature. The result is shown in Figure S1. It can be seen that at even at a temperature of T=462.5 K (189.5 C), less than 0.1% of the sample mass had been lost. As the evaporation temperatures are in the range 373-393 K (see Section 2 of the text), there is a safe margin in our experimental conditions.
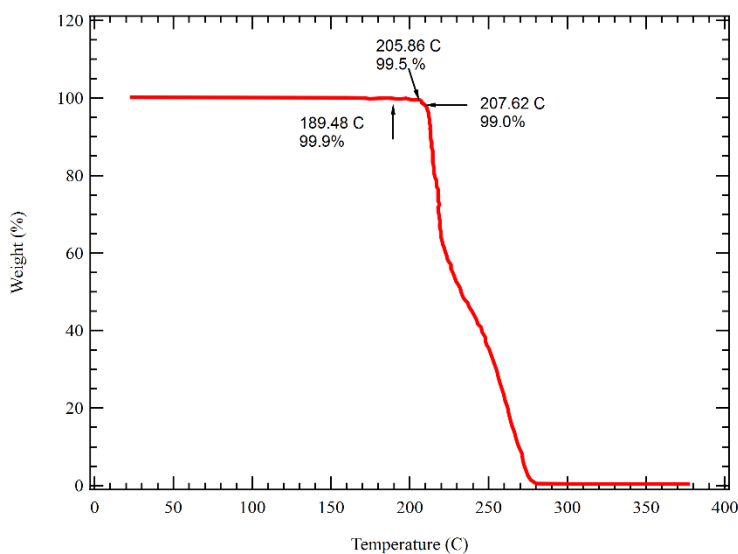

Figure S1. Thermogravimetric (TGA) measurements of the change of mass of a L-dialanine sample as a function of temperature.[1] Note the sharp onset of the mass decrease at 481 K.

S2. Defects on the Cu(100) surface

Copper has a relatively low stacking-fault energy and, consequently, these defects are abundant even in carefully grown single crystals.[2] Stacking-faults in FCC crystals are present on compact {111} planes and are encompassed by partial Shockley dislocations with Burgers vector of the type $\frac{a}{6}$ <112>, where a is the cubic cell parameter (see Figure S2).
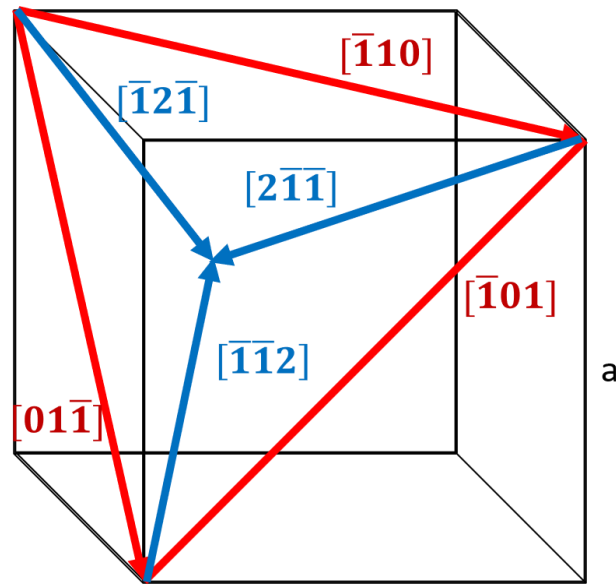

Figure S2. Thomson's tetrahedron inserted in the cube. In red the directions of the Burgers vector of perfect dislocations $\frac{a}{2}\langle 110 \rangle$, in blue directions of partial Shockley dislocations $\frac{a}{6}\langle 112 \rangle$. The three red lines along <110> define the (111) compact face of the crystal.

Let us take, as an example, the Shockley $\frac{a}{6}[\bar{1}2\bar{1}]$ on the (111) face. Its component parallel to the surface is $\boldsymbol{b}_\parallel = \frac{a}{6}[\bar{1}20]$. The equations for the elastic displacement field **u** around an edge dislocation lying along the x_3 direction, with Burgers vector b along x_1, are given by Friedel[3]:

$$u_1 = \frac{b}{2\pi}\left(\theta + \frac{\sin 2\theta}{4(1-v)}\right)$$

$$u_2 = -\frac{b}{2\pi}\left(\frac{1-2v}{2(1-v)}\log r + \frac{\cos 2\theta}{4(1-v)}\right)$$

where $\theta = \arctan(x_2/x_1)$ and $r = \sqrt{x_1^2 + x_2^2}$, v being the Poisson ratio. Transforming

the coordinates for a Burgers vector along $[\bar{1}20]$ we can fix the positions of the copper

(001) surface atoms around such a dislocation. A map of these positions is shown as

black points in Figure S3a where the trace of the direction, the projection of the

dislocation Burgers vector parallel to the surface, has also been represented. One can

see that there is a misfit of the [110] Cu atom rows when crossing a line which is the

parallel to the projection of the Burgers vector.
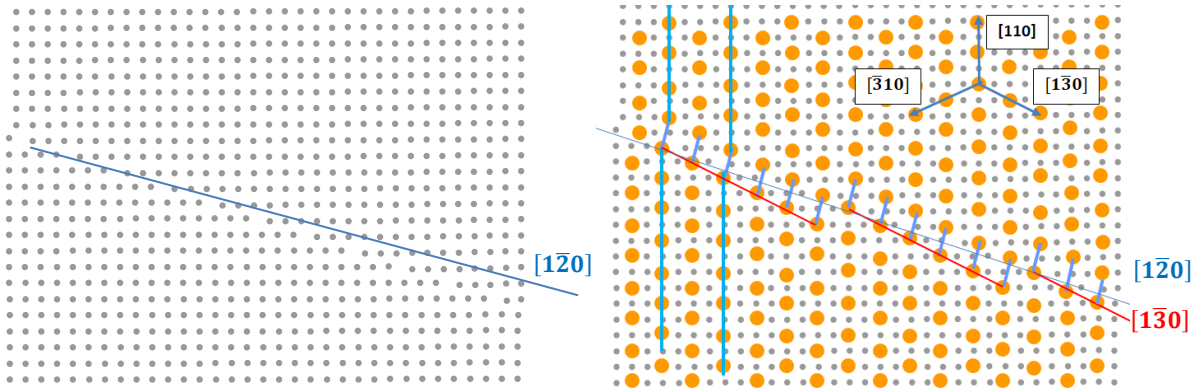

Figure S3. (a) Position of Cu atoms (black points) on a Cu(001) face in which a

Shockley partial dislocation with Burgers vector $\boldsymbol{b} = \frac{a}{6}[\bar{1}2\bar{1}]$ is present. The direction

of the projection of **b** on the surface along $[\bar{1}20]$ is shown by a blue line. (b) Dialanine

molecules (yellow disks) adsorbed on the Cu surface of Figure S3a in a c(2x4) structure.

Molecules rows along [110] directions are marked with thick blue lines. Note the lateral

shift of molecules across a misfit line of and compare with the experimental STM image

of Figure 5a. Note that the segments linking the molecules on the same side of the

misfit line consist of steps along $[\bar{1}30]$ whereas the enveloping line of the steps (in blue) is along $[\bar{1}20]$.

To construct Figure S3b (this is the Figure 5b of the text), the positions of the dialanine molecules are superimposed to the Cu atoms preserving the c(2x4) structure. Note the corresponding lateral displacement in Figure S3b of the compact [110] rows of dialanine molecules (thick blue lines) when crossing the misfit line. In terms of simple dislocation theory this misfit corresponds to the projection of the Burgers vector of the dislocation parallel to the surface, $\lfloor b_{\parallel} \rfloor$. A straightforward calculation shows that, $\lfloor b_{\parallel} \rfloor = a\frac{\sqrt{5}}{6} = d_{110}\frac{\sqrt{10}}{6} = 0.53\ d_{110}$, where d_{110} is the distance between adjacent rows of Cu atoms along [110]. As the distance among [110] rows of molecules is twice that of the corresponding [110] rows of Cu atoms underneath, a value for the lateral shift perpendicular to the molecules rows along [110] is $0.5 \times 0.53\ d_{110}$ (about ¼ d_{110}). This value is in good agreement with the observations. In the same Figure S3b, if one draws straight lines linking the atoms on the same side of the misfit, one obtains a series of segments all along the compact $[1\bar{3}0]$ direction forming a sawtooth line. The envelope of this line lies indeed along $[1\bar{2}0]$ in excellent agreement with the experiment.

References of the Supplementary Information

(1) The TGM measurements were performed by A. de la Escosura in the Department of Organic Chemistry of the Universidad Autónoma de Madrid.

(2) J.P, Hirth and J. Lothe, *Theory of Dislocations*; Mc Graw-Hill: New York 1968; Chapter 10.

(3) J. Friedel, *Dislocations*; Pergamon: Oxford 1967; page 20.