Supplementary material:
A new complex intermetallic phase in the system Al–Cu–Ta with familiar clusters and packing principles

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1. Diffuse scattering

The reconstructed diffuse scattering of a $hP386$-$Al_{57.4}Cu_{3.6}Ta_{39.0}$-crystal is shown in the figures below. The experimentally measured and the modeled diffuse scattering are compared, in which the Bragg intensities are not shown. It should be noted, that the measured crystal contained some impurities, which can be seen in the form of additional reflections in the reconstructions. The hnl-planes for $n = 0$ up to $n = 11$ are shown in Figs. 1–12.
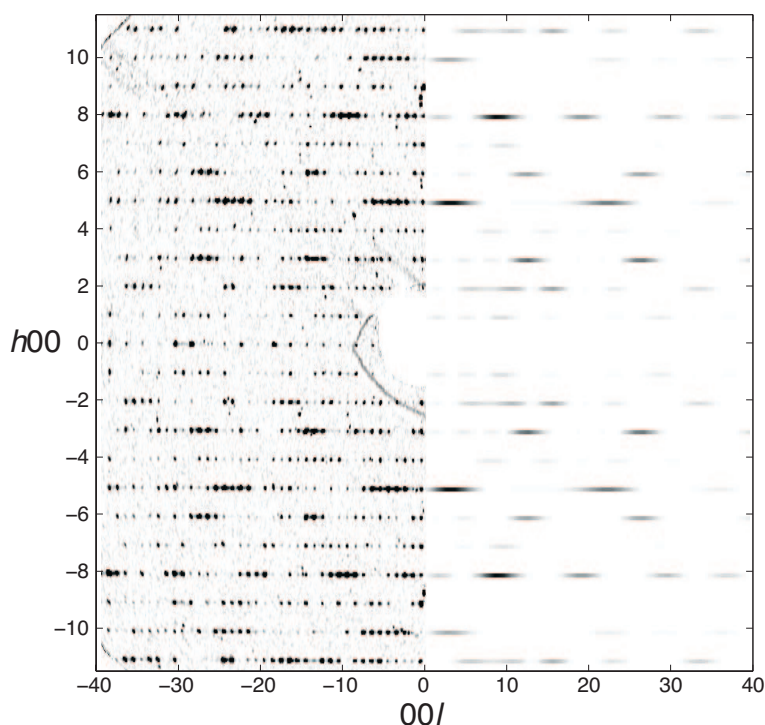

Figure 1
Measured *(left)* and calculated diffuse scattering *(right)* of the disordered single-crystal sample – $h0l$-plane.
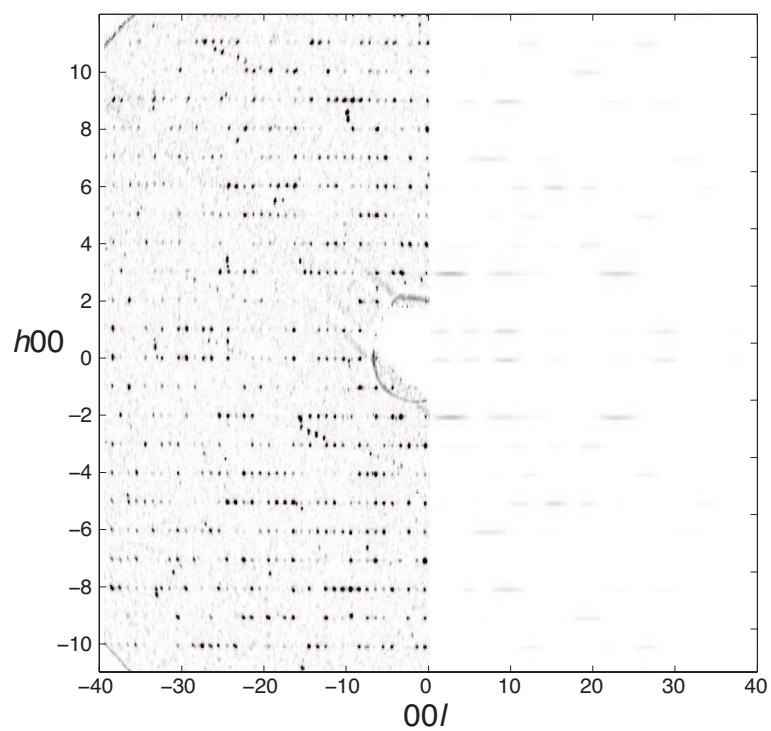
Figure 2
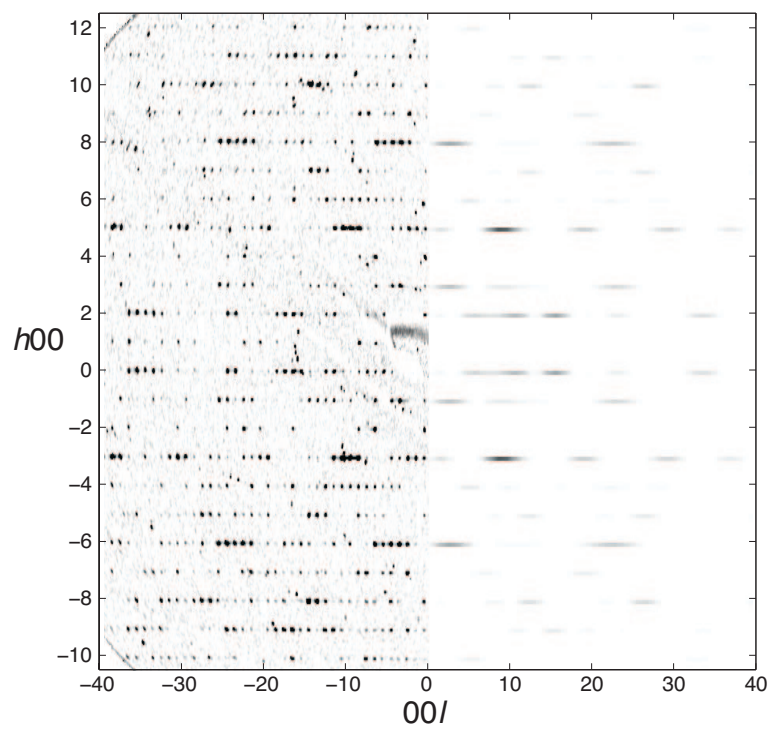Measured *(left)* and calculated diffuse scattering *(right)* of the disordered single-crystal sample – *h*1*l*-plane.

Figure 3
Measured *(left)* and calculated diffuse scattering *(right)* of the disordered single-crystal sample – *h*2*l*-plane.
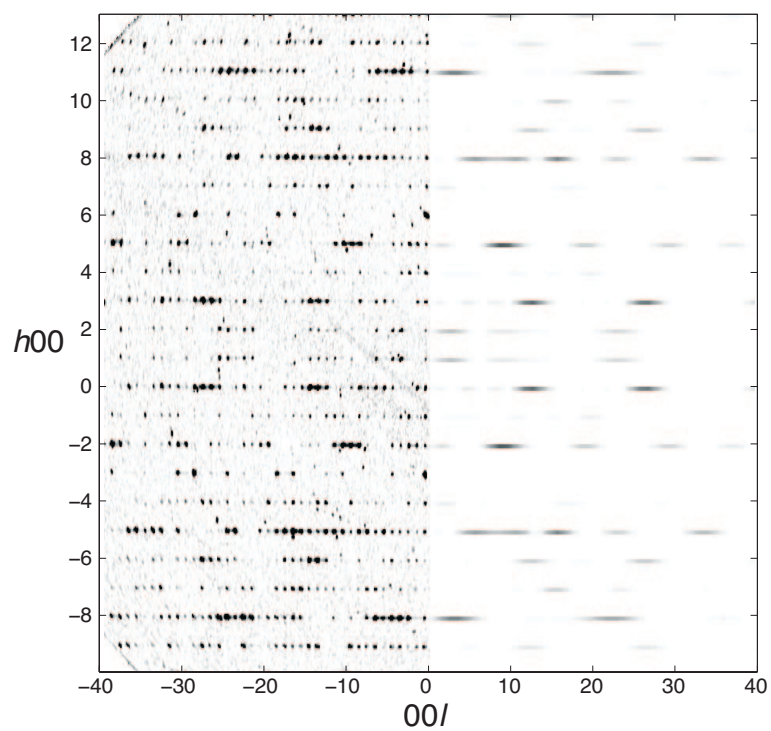
Figure 4
Measured *(left)* and calculated diffuse scattering *(right)* of the disordered single-crystal sample – *h3l*-plane.
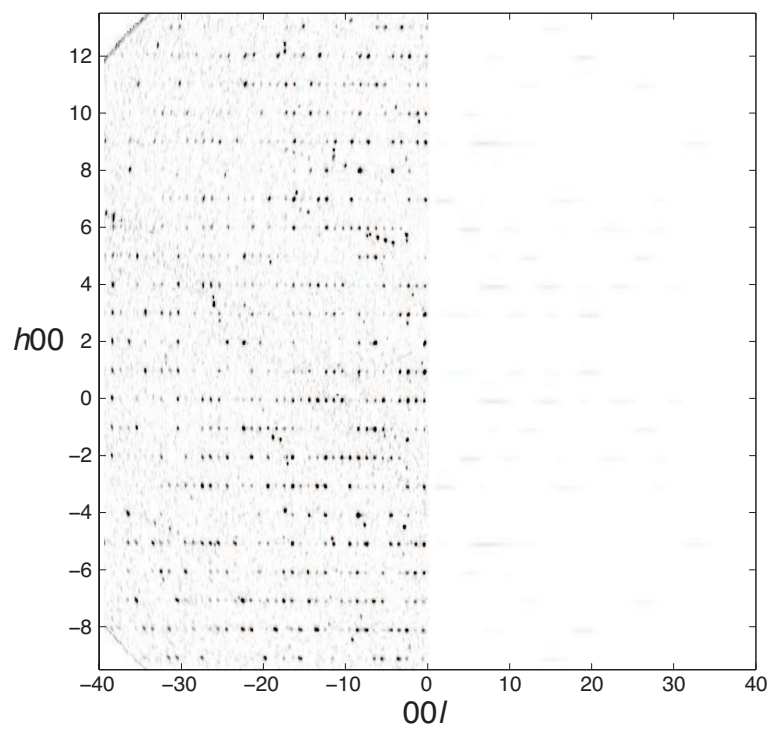

Figure 5
Measured *(left)* and calculated diffuse scattering *(right)* of the disordered single-crystal sample – *h4l*-plane.
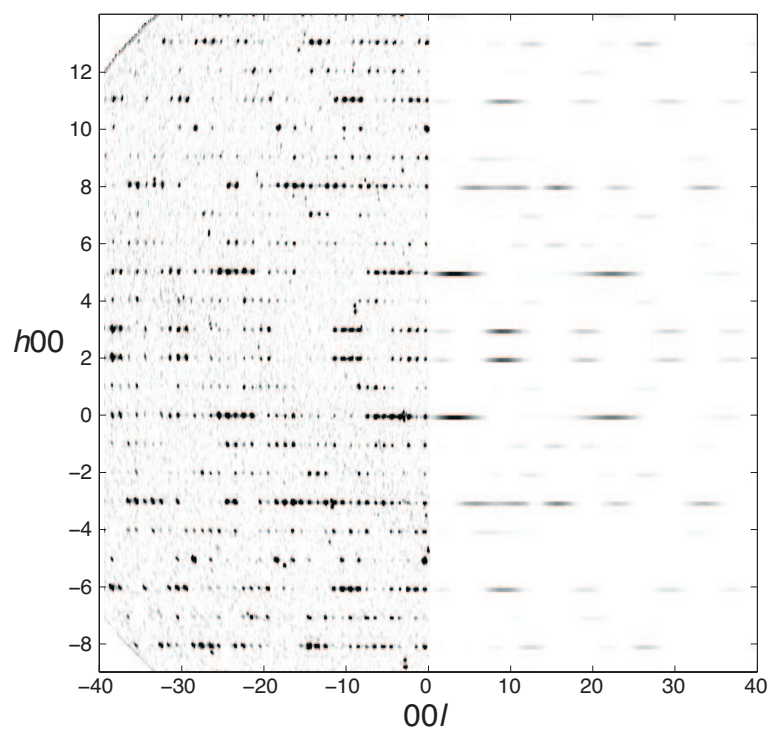
Figure 6
Measured *(left)* and calculated diffuse scattering *(right)* of the disordered single-crystal sample – *h5l*-plane.
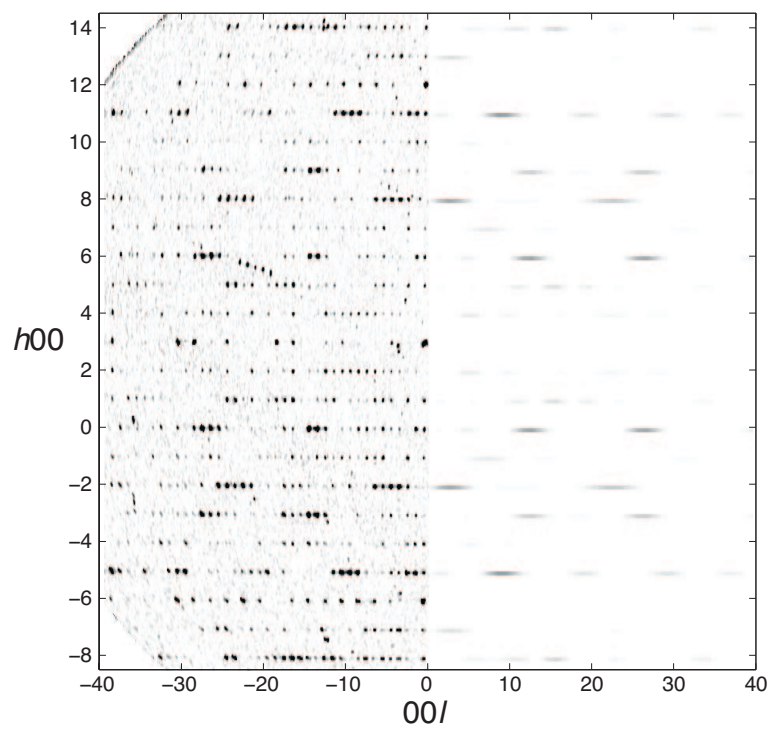

Figure 7
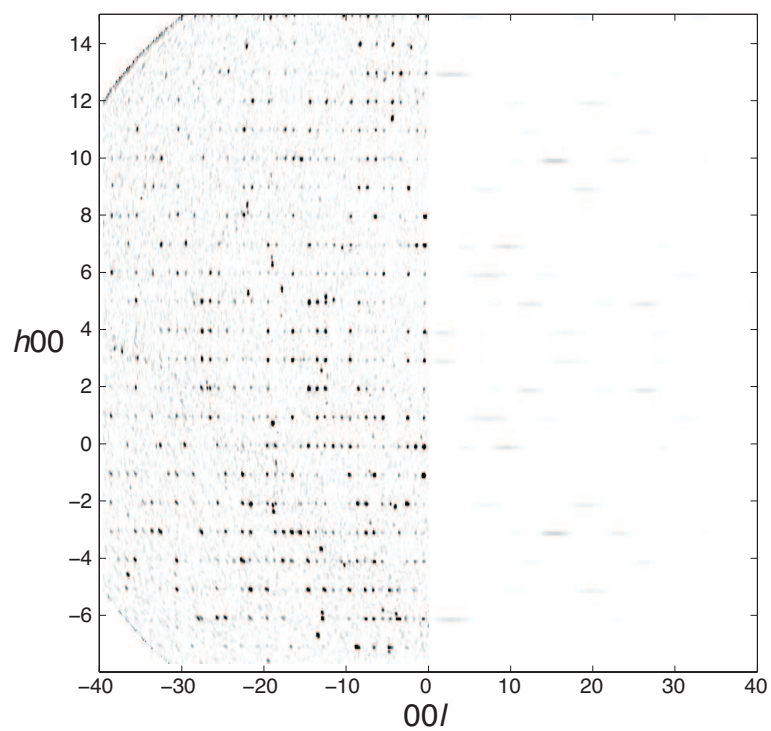Measured *(left)* and calculated diffuse scattering *(right)* of the disordered single-crystal sample – *h6l*-plane.

Figure 8
Measured *(left)* and calculated diffuse scattering *(right)* of the disordered single-crystal sample – *h*7*l*-plane.
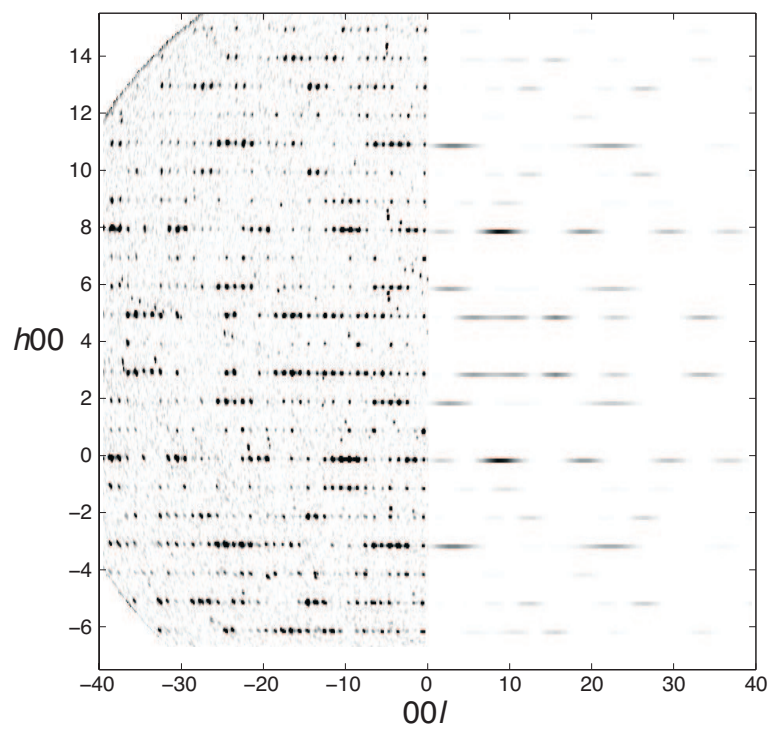

Figure 9
Measured *(left)* and calculated diffuse scattering *(right)* of the disordered single-crystal sample – *h*8*l*-plane.
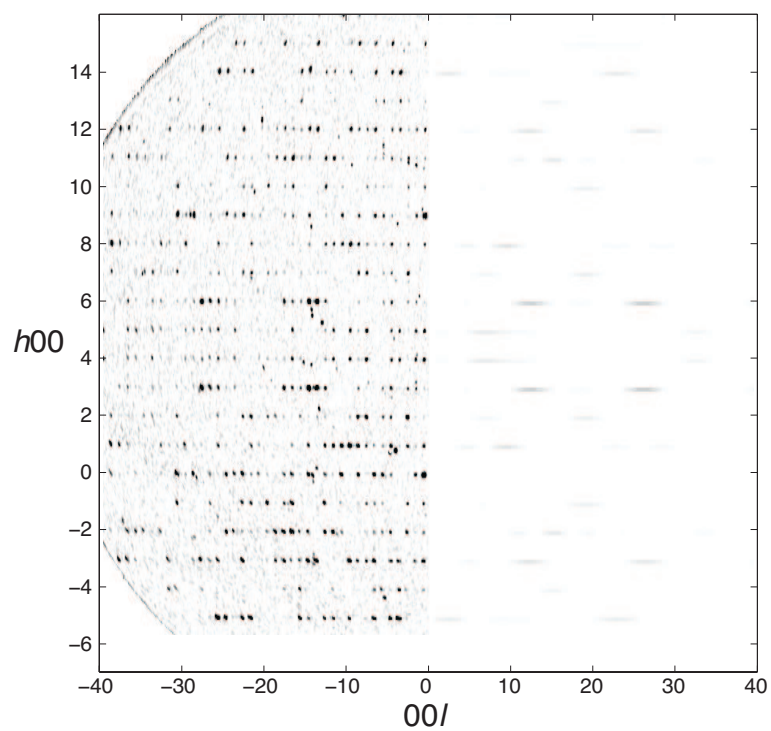
Figure 10
Measured *(left)* and calculated diffuse scattering *(right)* of the disordered single-crystal sample – *h9l*-plane.
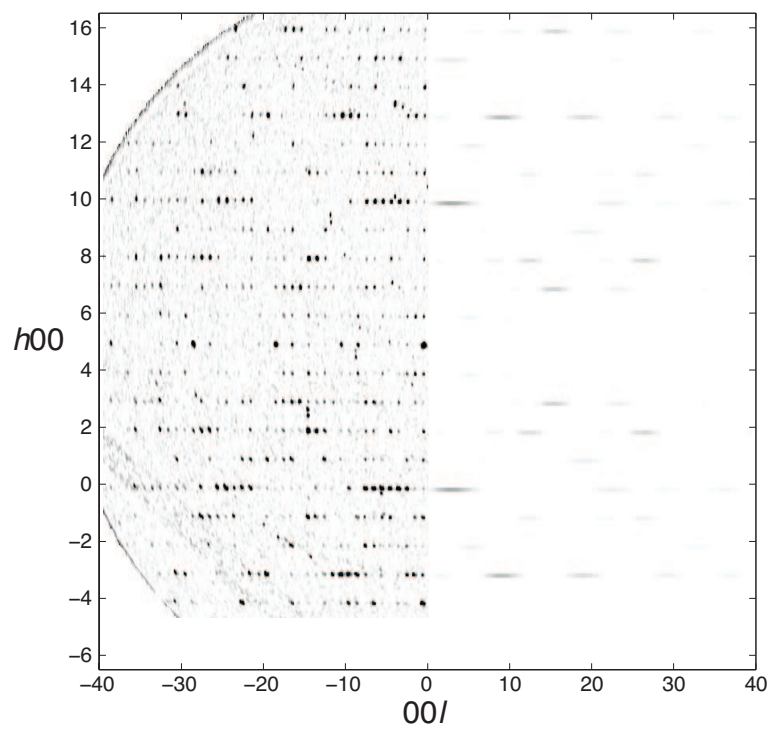

Figure 11
Measured *(left)* and calculated diffuse scattering *(right)* of the disordered single-crystal sample – *h10l*-plane.
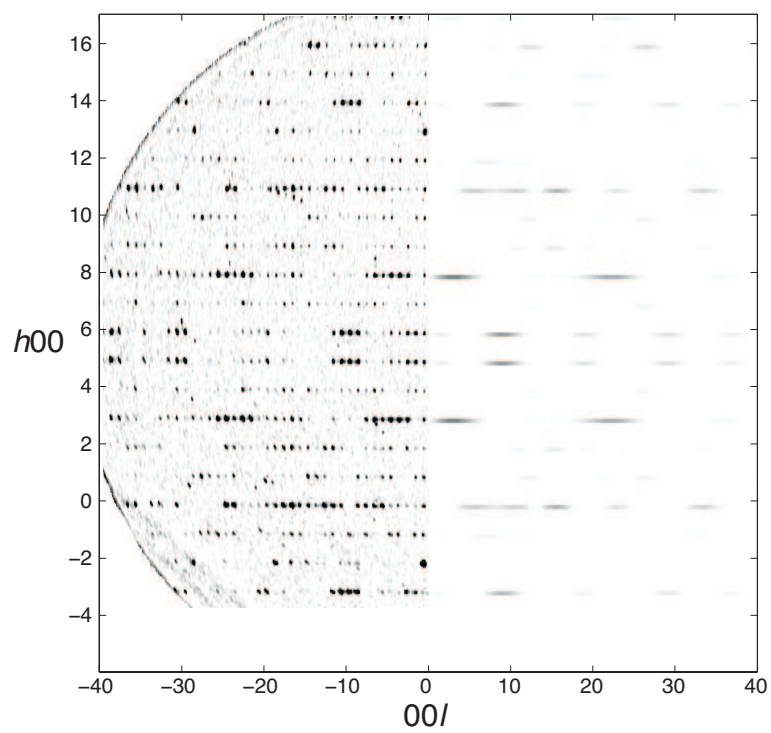
Figure 12
Measured *(left)* and calculated diffuse scattering *(right)* of the disordered single-crystal sample – *h*11*l*-plane.
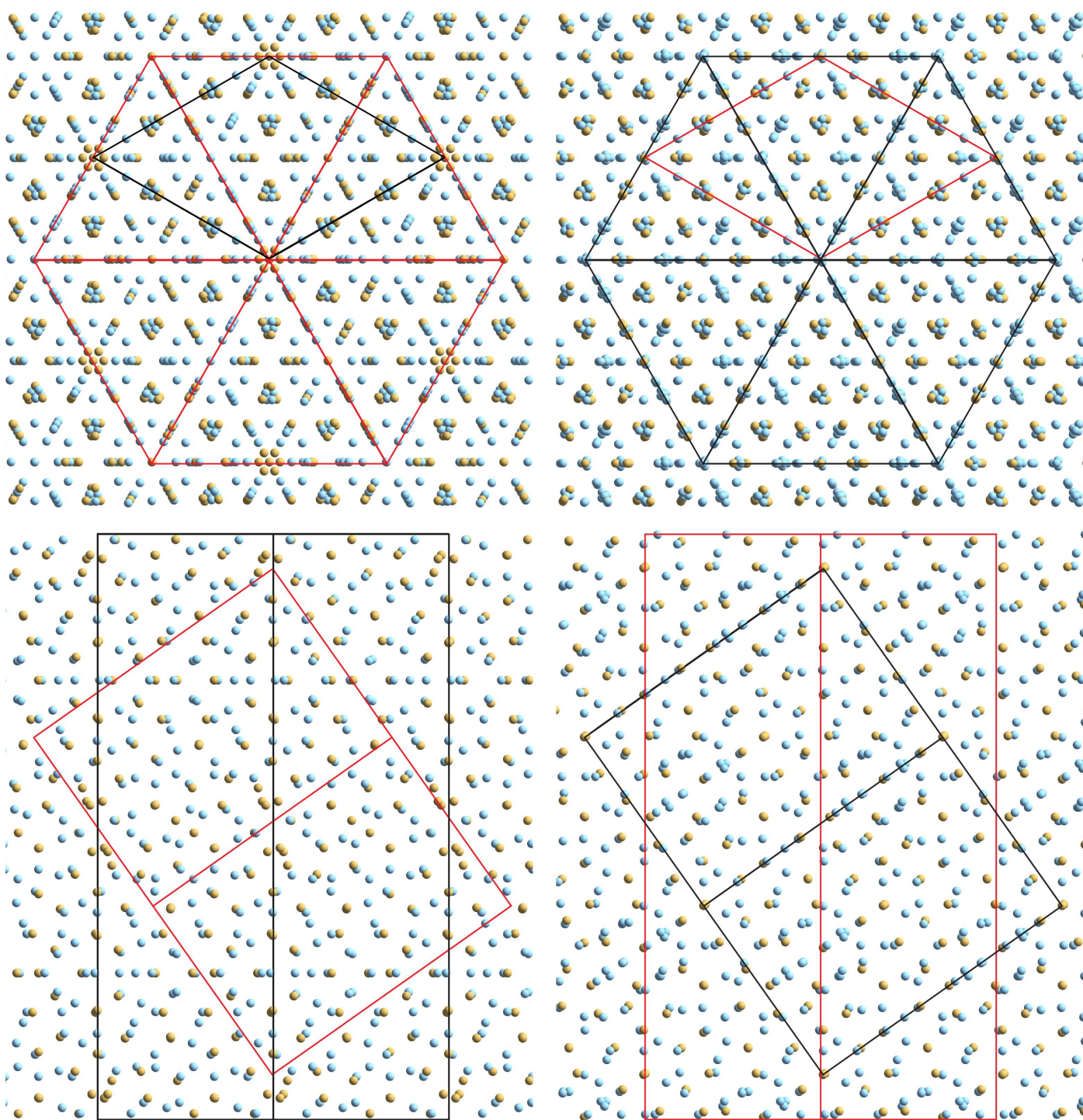
2. Layer structure

Figure 13
Projections of the structures $hP386$-$Al_{57.4}Cu_{3.6}Ta_{39.0}$ *(left)* and $cF444$-$Al_{63.6}Ta_{36.4}$ *(right)*. The projections are prepared along the $[001]$- and $[111]$-directions, respectively *(top)*, rendering very similar views for the hexagonal and cubic structure along the 6_3- and 3-axes, respectively. In addition, the views perpendicular to the projections on the top are shown, projected along the $[110]$- and $[\bar{1}01]$-directions *(bottom)*. The unit cells are outlined in black, respectively, while the red contour delineates the unit cell of the other structure, respectively.