Electronic Supplementary Information

Chemical Epitaxy of a New Orthorhombic Phase of $Cu_{2-x}S$ on GaAs

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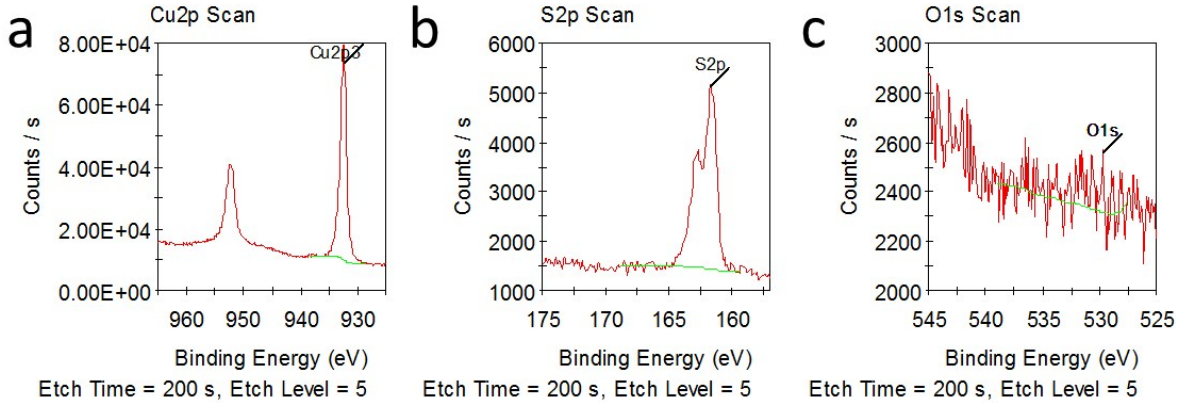

Fig. S1 High-resolution XPS of etched $Cu_{2-x}S$ thin films deposited on GaAs(100). Cu with 2p3 photoelectron peaks indicate binding energies of 932.5 eV and 952.3 eV (b) S - 2p photoelectron peak show binding energies of 161.7 eV and 162.8 eV. (c) O – 1s photoelectron peak is indistinguishable.

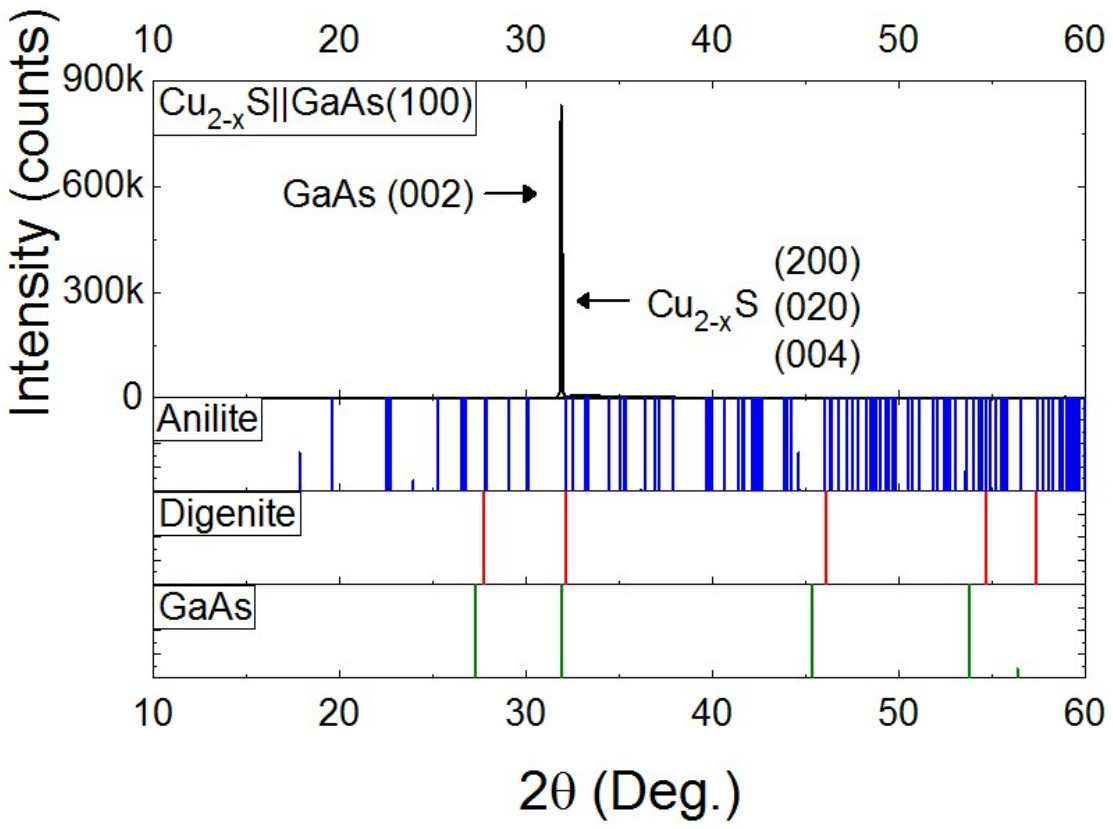

Fig. S2 Wide 2θ range X-ray diffractogram of $Cu_{2-x}S$ thin films deposited on GaAs(100) at temperature of 70℃ for growth duration of 5 hr, $Cu_{2-x}S$ – Anilite (1251523, Pearson's crystal data), $Cu_{2-x}S$ - Digenite (455552 , Pearson's crystal data) and GaAs – zinc blende (453930, Pearson's crystal data). See Fig.3 in main text for a magnified and resolved view of the region 2θ≈32 degrees.

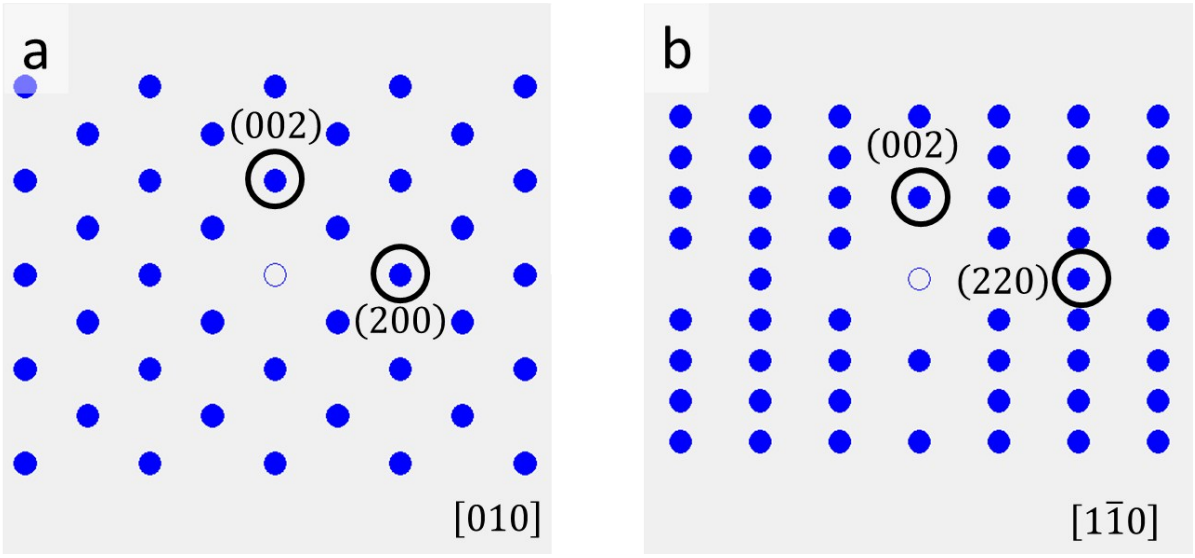

Fig. S3 Simulated electron diffraction patterns of Anilite phase (1251523, Pearson's crystal data) along zone axes: (a) [010] and (b) [1$\bar{1}$0].

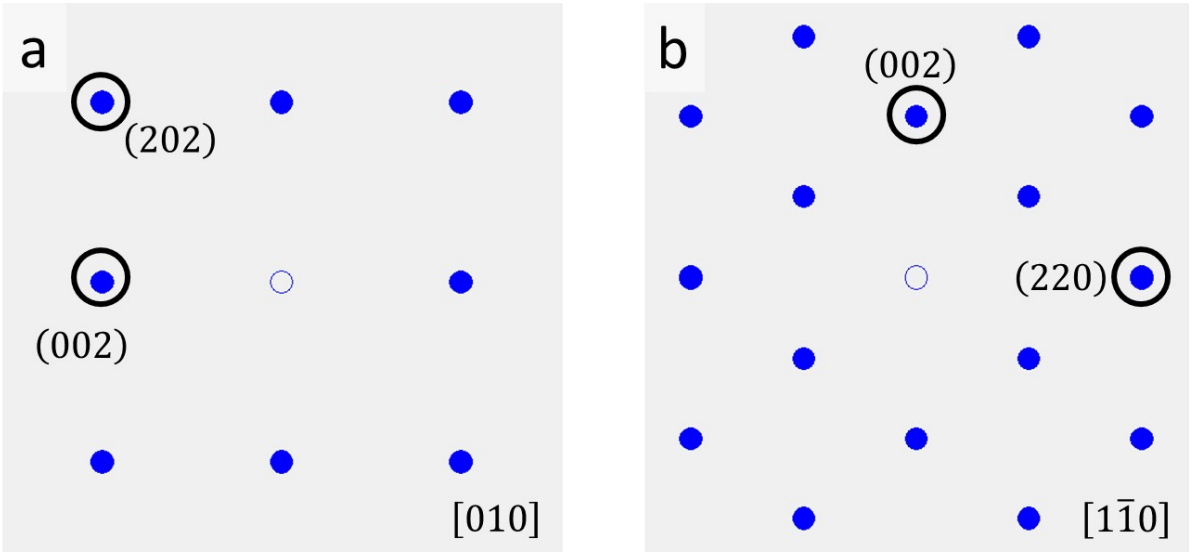

Fig. S4 Simulated electron diffraction patterns of Digenite phase (455552, Pearson's crystal data) along zone axes: (a) [010] and (b) [1$\bar{1}$0].

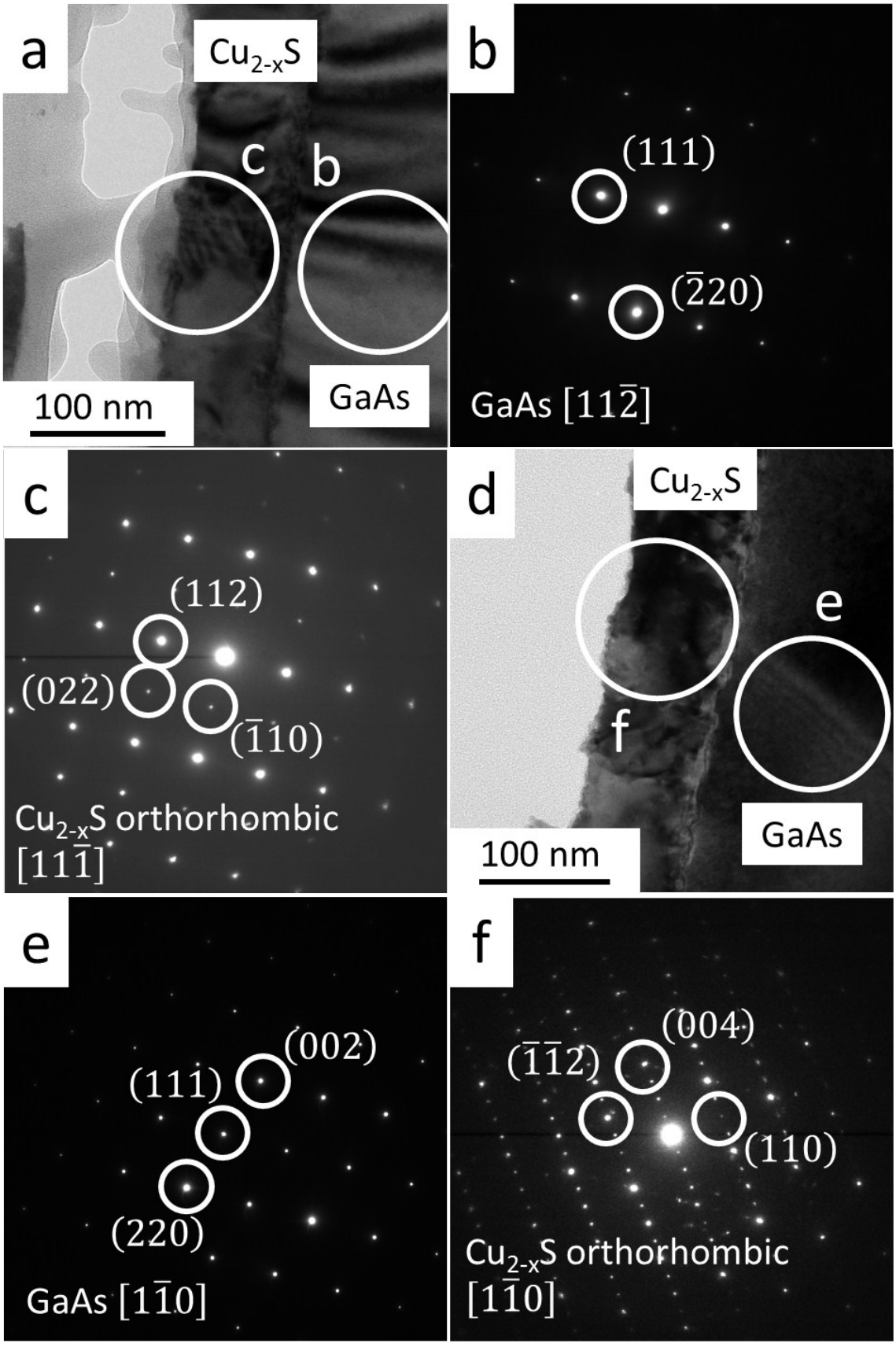
a
$Cu_{2-x}S$
c
b
100 nm
GaAs
b
(111)
$(\bar{2}20)$
GaAs $[11\bar{2}]$
c
(112)
$(02\bar{2})$
$(\bar{1}10)$
$Cu_{2-x}S$ orthorhombic
$[11\bar{1}]$
d
$Cu_{2-x}S$
e
f
100 nm
GaAs
e
(002)
(111)
(220)
GaAs $[1\bar{1}0]$
f
(004)
$(\bar{1}\bar{1}2)$
$(1\bar{1}0)$
$Cu_{2-x}S$ orthorhombic
$[1\bar{1}0]$

Fig. S5 (a) Cross-sectional BF-TEM image of $Cu_{2-x}S$ film deposited on GaAs(111)A at deposition temperature of 70˚C for growth duration of 5 hr. (b) SAED pattern taken from the area marked with a white circle in "b", indicating GaAs $[11\bar{2}]$ ZA. (c) SAED pattern taken from the area marked with a white circle in "c", indicating $Cu_{2-x}S$ $[11\bar{1}]$ ZA. (d) 90° rotated cross-sectional BF-TEM micrograph of $Cu_{2-x}S$ film. (e) SAED pattern taken from region marked with "e" in the BF-TEM micrograph, indicating GaAs $[1\bar{1}0]$ ZA. (f) SAED pattern taken from region marked "f" in the BF-TEM micrograph, indicating BCO phase $Cu_{2-x}S$ film in ZA of $[1\bar{1}0]$.

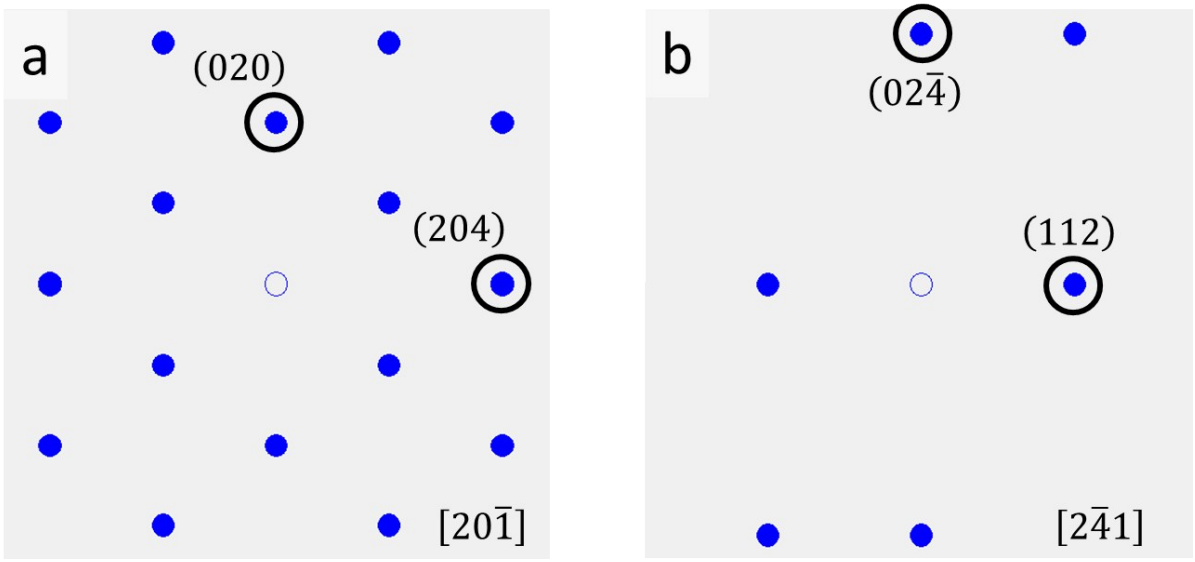

Fig. S6 Simulated electron diffraction patterns of base-centered orthorhombic (BCO) $Cu_{2-x}S$ phase with lattice parameters a ≈ b = 5.6 Å and c = 11.2 Å viewed along zone axes $[20\bar{1}]$ and $[2\bar{4}1]$.