metals

MDPI

*Article*

# Crystal Structures of $Al_2Cu$ Revisited: Understanding Existing and Exploring Potential Phases

**Sai Wang and Changzeng Fan ***

State Key Laboratory of Metastable Materials Science and Technology, Yanshan University, Qinhuangdao 066004, China; wangsxcmg@163.com

* Correspondence: chzfan@ysu.edu.cn; Tel.: +86-335-805-7047

Received: 5 August 2019; Accepted: 14 September 2019; Published: date

**Table 1.** Crystal data, data collection and structure refinement details of the pseudo $Al_2Cu$ phase.

| Crystal data | Values |
|---|---|
| Chemical formula | $Al_{1.97}Cu$ |
| $M_r$ | 116.77 |
| Crystal system, space group | Tetragonal, *P4/mmm* |
| Temperature (K) | 293 |
| *a*, *c* (Å) | 4.279 (2), 2.4337 (13) |
| *V* (Å$^3$) | 44.56 (5) |
| *Z* | 1 |
| Radiation type | Mo *Kα* |
| μ (mm$^{-1}$) | 12.64 |
| Data collection Diffractometer | Bruker D8 Venture Photon 100 CMOS |
| Data processing programs | APEX3, SAINT and SADABS [1]; SHELXT [2]; SHELXL2014/7 [3]. |
| Absorption correction | Multi-scan |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 1283, 51, 50 |
| $R_{int}$ | 0.068 |
| $(\sin\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.665 |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S* | 0.022, 0.050, 1.11 |
| No. of unique reflections | 51 |
| No. of parameters | 8 |
| Δρmax, Δρmin (e Å$^{-3}$) | 0.53, −1.35 |

**Table 2.** Crystallographic information of all existing $Al_2Cu$ phases (the Owen-, θ-, θ'- and Ω phase) and two proposed potential $Al_2Cu$ phases (M1 and M2 phase) corresponding to the available cif files.

| Phase | Space Group | | Lattice Parameters | | | Wyckoff positions | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | Symbol | number | *a* | *b* | *c* | Atom site | | *x* | *y* | *z* |
| Owen | *P4/mmm* | 123 | 4.28 | 4.28 | 2.405 | Al1 | 2*e* | 1/2 | 0 | 1/2 |
| | | | | | | Cu1 | 1*a* | 0 | 0 | 0 |
| Ω | *Fmmm* | 69 | 4.96 | 8.59 | 8.48 | Al1 | 8*h* | 0 | 1/3 | 0 |
| | | | | | | Al2 | 8*i* | 0 | 0 | 1/6 |
| | | | | | | Cu1 | 8*f* | 1/4 | 1/4 | 1/4 |
| θ | *I4/mcm* | 140 | 6.067 | 6.067 | 4.877 | Al1 | 8*h* | 0.1581 | 0.6581 | 0 |
| | | | | | | Cu1 | 4*a* | 0 | 0 | 1/4 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| θ' | *I4/mmm* | 139 | 4.04 | 4.04 | 5.80 | Al1 | 4*d* | 1/2 | 0 | 1/4 |
| | | | | | | Cu1 | 2*a* | 0 | 0 | 0 |
| M1 | *I4/mcm* | 140 | 6.047 | 6.047 | 10.052 | Al1 | 16*l* | 0.8405 | 0.3405 | 0.1355 |
| | | | | | | Cu1 | 4*c* | 0 | 0 | 1/2 |
| | | | | | | Cu2 | 4*a* | 0 | 0 | 1/4 |
| M2 | *I4/mcm* | 140 | 6.008 | 6.008 | 15.445 | Al1 | 16*l* | 0.3406 | 0.8406 | 0.3244 |
| | | | | | | Al2 | 8*h* | 0.3320 | 0.8320 | 1/2 |
| | | | | | | Cu1 | 8*f* | 1/2 | 1/2 | 0.9154 |
| | | | | | | Cu2 | 4*a* | 1/2 | 1/2 | 3/4 |
| Pseudo | *P4/mmm* | 123 | 4.275 | 4.275 | 2.431 | Al1 | 4*l* | 0.3159 | 0 | 0 |
| | | | | | | Cu1 | 1*d* | 1/2 | 1/2 | 1/2 |

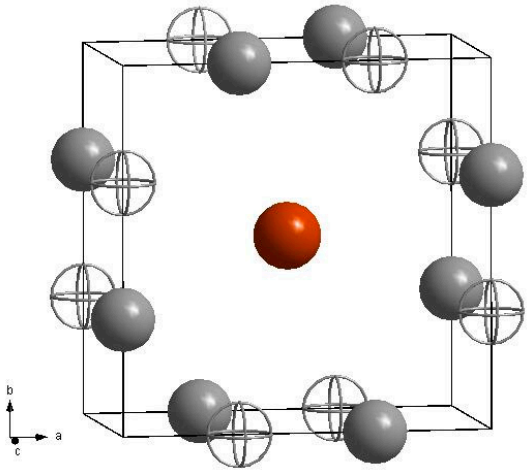
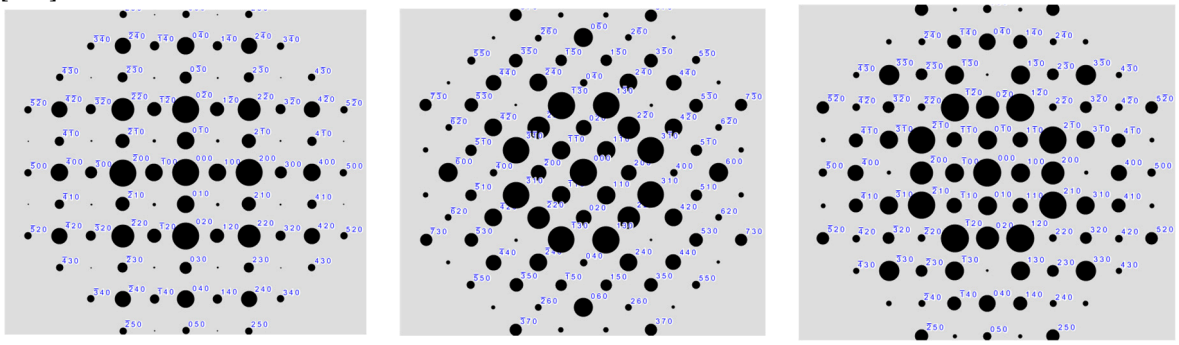
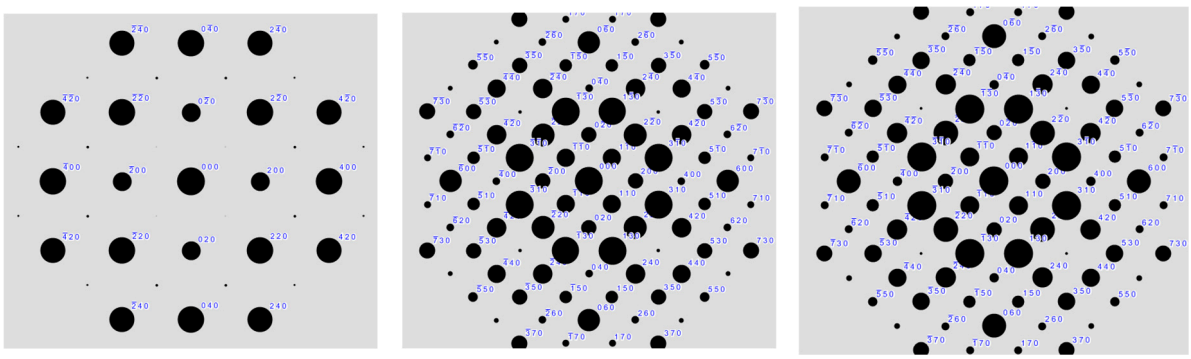



**Figure 1.** The structural model of the pseudo $Al_2Cu$ phase (The Cu atoms are indicated in brown color balls; Owing to the close Al-Al connections along the edges thus cannot occupied simultaneously, the Al atoms are represented by filled gray and empty white spheres).

[100]

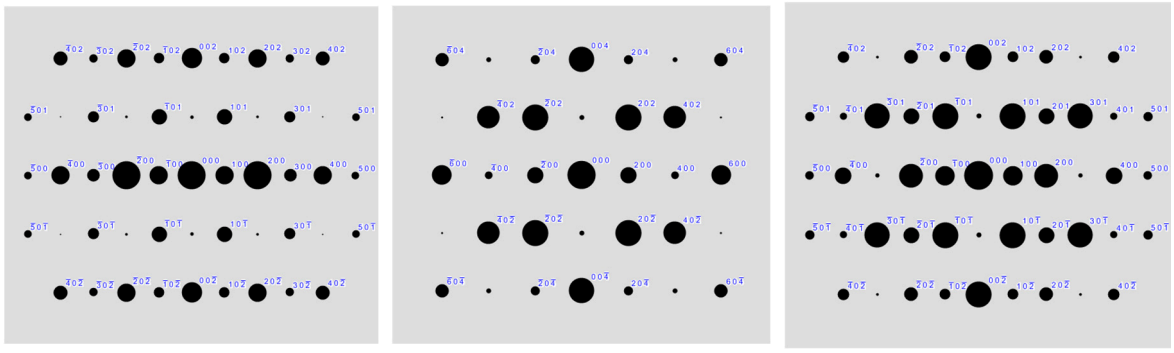


Owen θ Ω

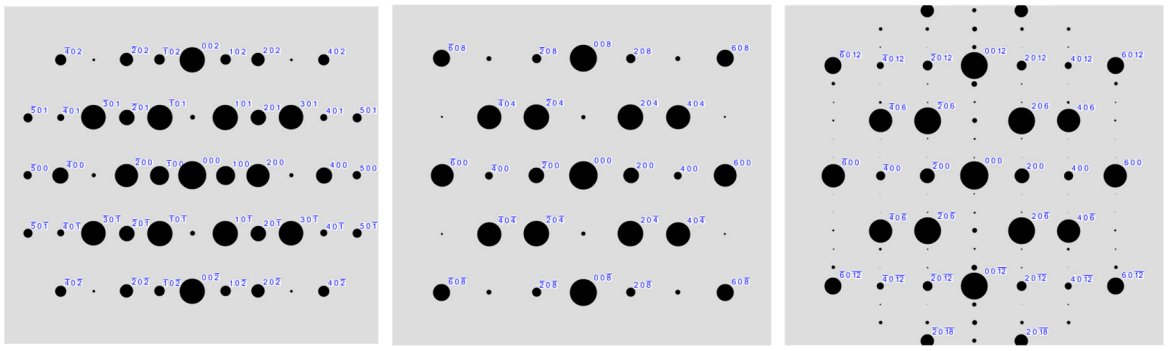


θ′ M1 M2

[010]

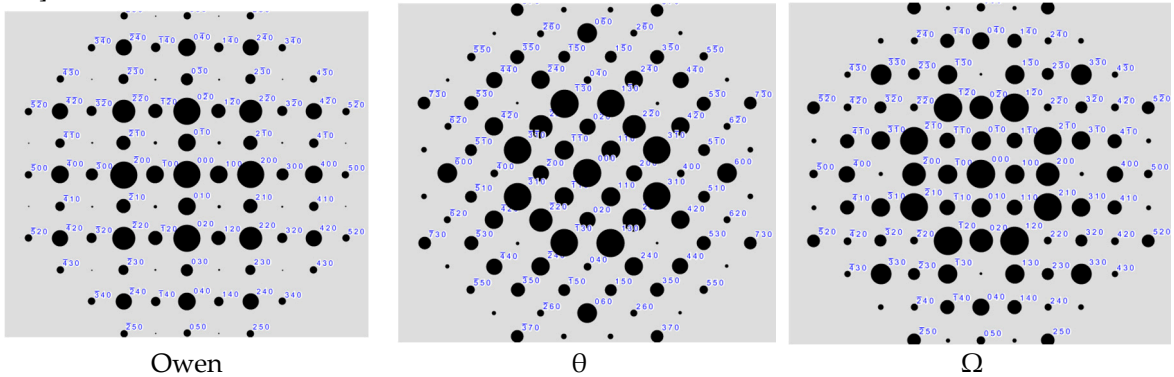


Owen θ Ω



θ′ M1 M2

[001]



Owen θ Ω

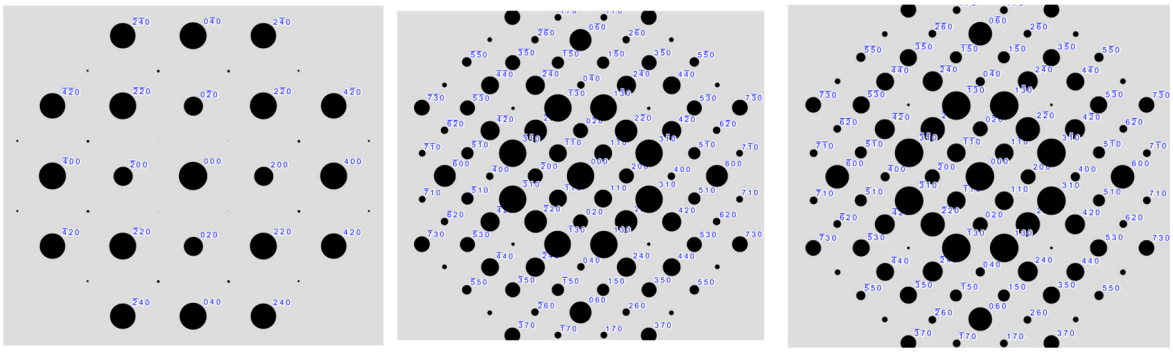



**Figure 2.** Projected simulated single crystal diffraction patterns of all existing and potential phases along [100], [010] and [001] directions.

[1] APEX3, SAINT and SADABS. Software for data reduction, absorption correction and structure solution. Bruker AXS Inc. Madison, Wisconsin, USA. (2015).

[2] Sheldrick, G. M. SHELXT: Integrating space group determination and structure solution. *Acta Cryst*. 2015, A71, 3-8.

[3] Sheldrick, G. M. Crystal structure refinement with SHELXL. *Acta Cryst*. 2015, C71, 3-8.