# $U_{1.33}T_4Al_8Si_2$ (T = Ni, Co): Complex uranium silicides grown from aluminum/gallium flux mixtures

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## Supporting Information

**Figure S1.** Microscope images of flux-grown uranium silicides. (a) Pencil-shaped $U_{1.33}Co_4Al_8Si_2$ crystals. (b) $U(Al/Ga/Si)_3$ crystals that form as a byproduct in reactions of U/Ni/Si in Ga/Al flux.

**Figure S2.** X-ray powder diffraction pattern for products of the reaction of U/Ni/Si in Al/Ga flux (bottom), compared to calculated patterns for $U_{1.33}Ni_4Al_8Si_2$ and $U(Al/Si)_3$.

**Figure S3.** X-ray powder diffraction pattern for products of the reaction of U/Co/Si in Al/Ga flux, compared to calculated pattern for $U_{1.33}Co_4Al_8Si_2$.

**Figure S4.** EDS mapping of $U_{1.33}Ni_4Al_8Si_2$ crystal after TGA experiment (heated to 900°C in flowing air).

**Figure S5.** Thermogravimetric analysis of $U_{1.33}Co_4Al_8Si_2$ crystals heated in air, and microscope image of oxide coated crystals.

**Table S1.** Selected bond lengths (in Å) in the $U_{1.33}T_4Al_8Si_2$ structures (T = Ni or Co).

**Table S2**. Atomic percentages based on single crystal X-ray diffraction and SEM EDS for $U_{1.33}Ni_4Al_8Si_2$ compound.

**Table S3**. Atomic percentages based on single crystal X-ray diffraction and SEM EDS for $U_{1.33}Co_4Al_8Si_2$ compound.

**Table S4**. Atomic coordinates and site occupancies for $U_{1.33}Ni_4Al_8Si_2$ structure.

**Table S5**. Atomic coordinates and site occupancies for $U_{1.33}Co_4Al_8Si_2$ structure.

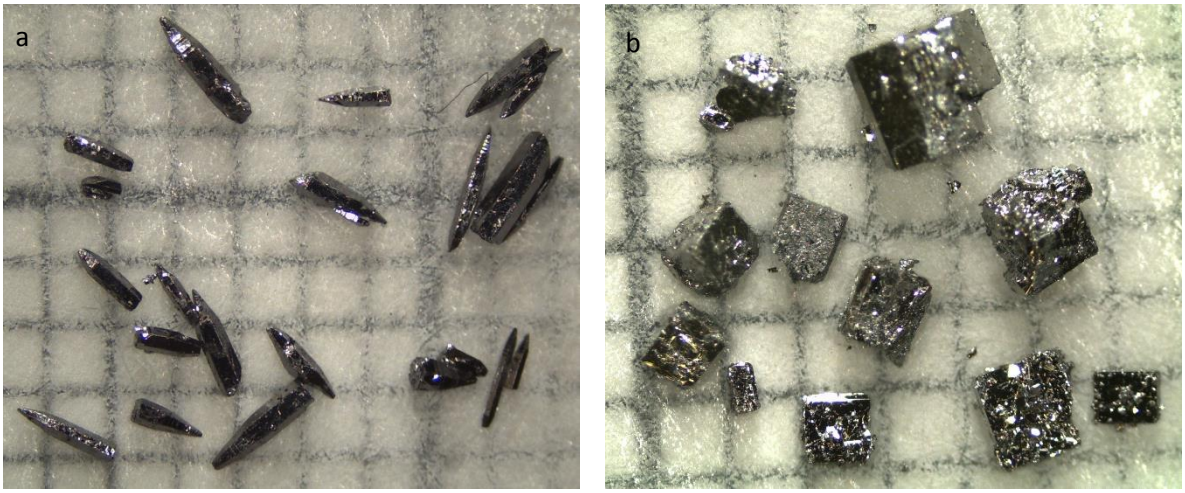



**Figure S1.** Microscope images of flux-grown uranium silicides. (a) Pencil-shaped $U_{1.33}Co_4Al_8Si_2$ crystals. (b) $U(Al/Ga/Si)_3$ crystals that form as a byproduct in reactions of U/Ni/Si in Ga/Al flux.

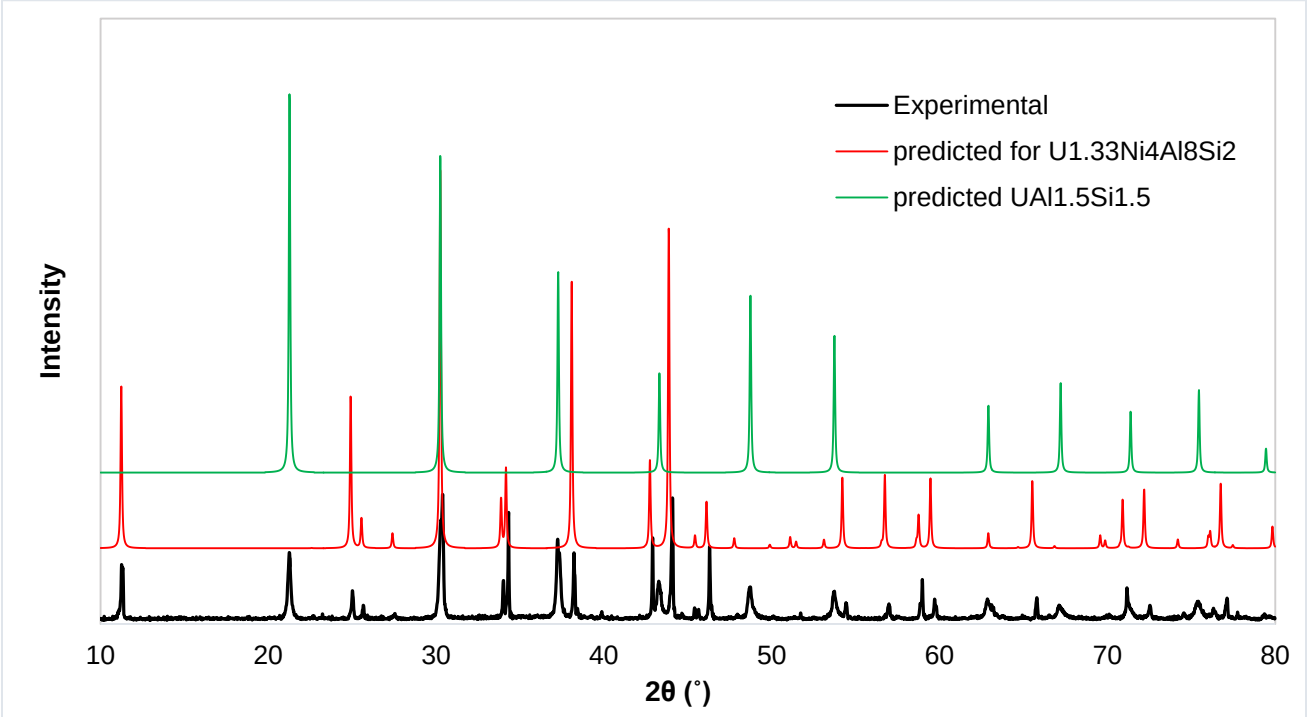



**Figure S2.** X-ray powder diffraction pattern for products of the reaction of U/Ni/Si in Al/Ga flux (bottom), compared to calculated patterns for $U_{1.33}Ni_4Al_8Si_2$ and $U(Al/Si)_3$.

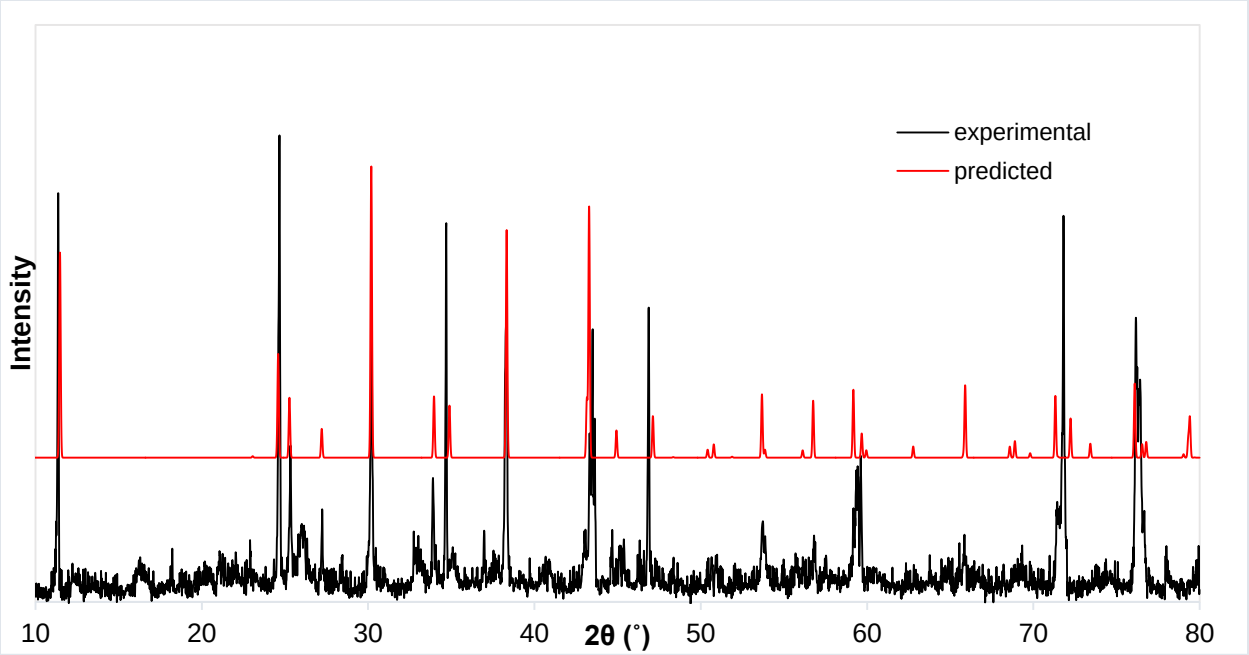
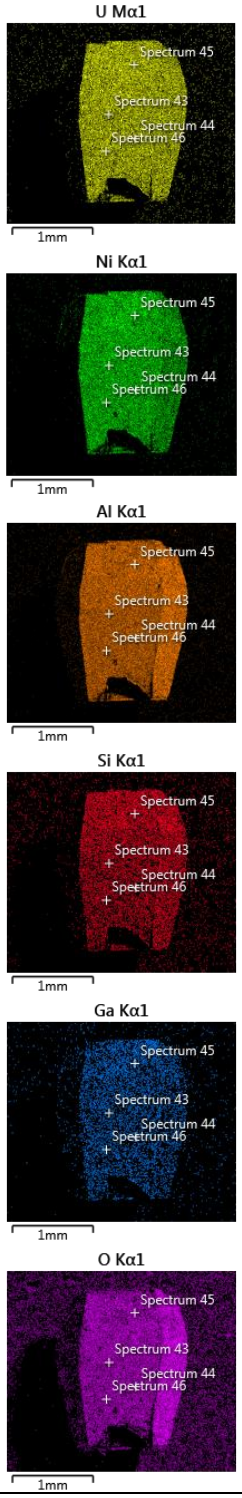
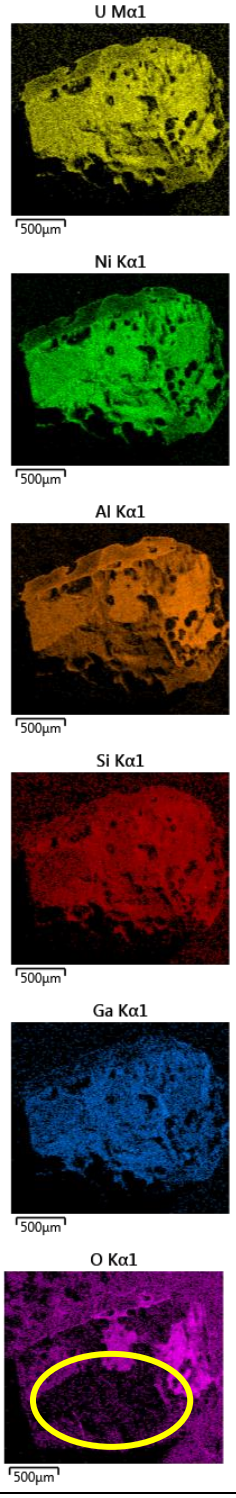



**Figure S3.** X-ray powder diffraction pattern for products of the reaction of U/Co/Si in Al/Ga flux, compared to calculated pattern for $U_{1.33}Co_4Al_8Si_2$.

| Post TGA $U_{1.33}Ni_4Al_8Si_2$ crystal | Interior of the same crystal after chipping a small piece |
|---|---|
|  |  |



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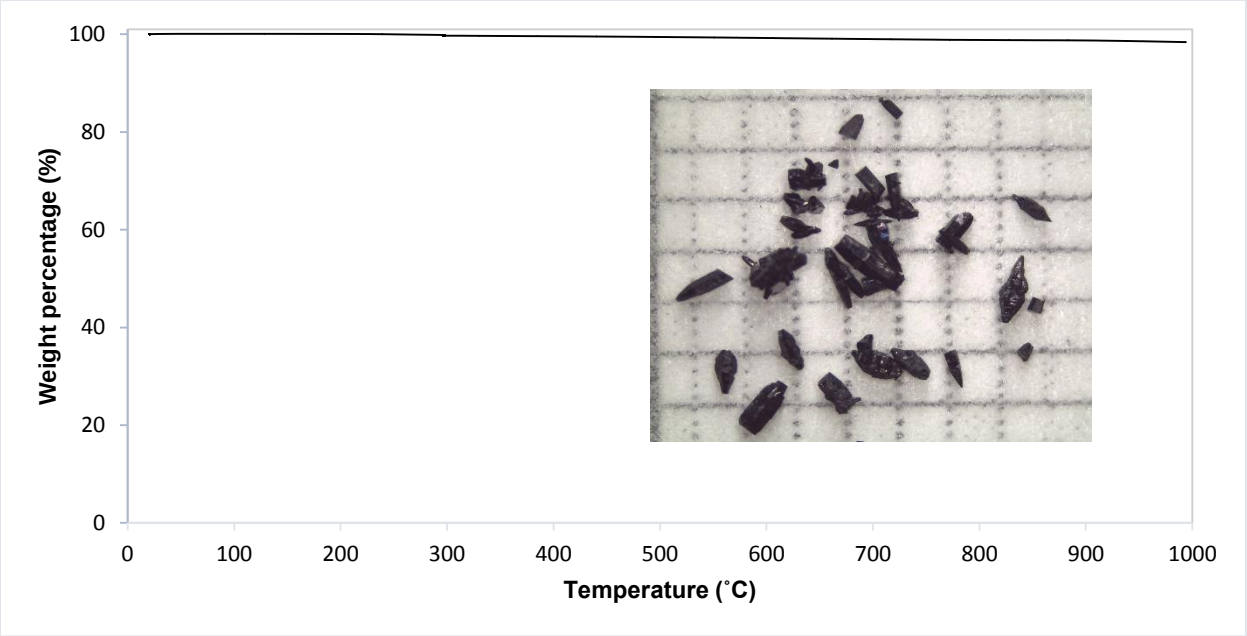


**Figure S5.** Thermogravimetric analysis of $U_{1.33}Co_4Al_8Si_2$ crystals heated in air, and microscope image of oxide coated crystals.

**Table S1.** Selected bond lengths (in Å) in the $U_{1.33}T_4Al_8Si_2$ structures (T = Ni or Co).

| | **$U_{1.33}Ni_4Al_8Si_2$** | **$U_{1.33}Co_4Al_8Si_2$** |
|---|---|---|
| U(1)-Si(1) | 2.986(5) | 2.900(3) |
| U(1)-Al(1) | 3.0036(13) | 2.9819(9) |
| T(1)-Si(1) | 2.397(3) | 2.3140(17) |
| T(1)-Al(1) | 2.4087(5) | 2.3534(4) |
| T(1)-Al(2) | 2.479(3) | 2.5721(8) |
| Al(1)-Al(2) | 2.7451(15) | 2.6991(12) |
| Al(1)-Si(1) | 2.7665(14) | 2.7557(10) |
| Si(1)-Si(1) | 2.448(11) | 2.474(6) |

**Table S2**. Atomic percentages based on single crystal X-ray diffraction and SEM EDS for $U_{1.33}Ni_4Al_8Si_2$ compound.

| | Atomic percentages based on single crystal formula (%) | Atomic percentages based on SEM/EDS (%) |
|---|---|---|
| U | 7 | 7(1) |
| Ni | 27 | 31(4) |
| Al | 51 | 41(4) |
| Si | 12 | 16(2) |
| Ga | 3 | 5(1) |

**Table S3**. Atomic percentages based on single crystal X-ray diffraction and SEM EDS for $U_{1.33}Co_4Al_8Si_2$ compound.

| | Atomic percentages based on single crystal formula (%) | Atomic percentages based on SEM/EDS (%) |
|---|---|---|
| U | 9 | 10(1) |
| Co | 26 | 25(5) |
| Al | 51 | 39(4) |
| Si | 13 | 19(3) |
| Ga | 1 | 7(2) |

**Table S4**. Atomic coordinates and site occupancies for $U_{1.33}Ni_4Al_8Si_2$ structure.

| Atom | Site | x | y | z | Occupancy |
|---|---|---|---|---|---|
| U1 | 2(c) | 1/3 | 2/3 | 1/4 | 0.526 |
| Ni1 | 4(f) | 1/3 | 2/3 | 0.61067(6) | 1 |
| Al1 | 4(e) | 0 | 0 | 0.1337(1) | 0.928 |
| Ga11 | 4(e) | 0 | 0 | 0.1337(1) | 0.072 |
| Al2 | 4(f) | 1/3 | 2/3 | 0.0469(1) | 1 |
| Si1 | 6(h) | 0.5311(9) | 0.062(2) | 1/4 | 0.300 |
| Ga1 | 6(h) | 0.5311(9) | 0.062(2) | 1/4 | 0.033 |

**Table S5**. Atomic coordinates and site occupancies for $U_{1.33}Co_4Al_8Si_2$ structure.

| Atom | Site | x | y | z | Occupancy |
|---|---|---|---|---|---|
| U1 | 2(c) | 1/3 | 2/3 | 1/4 | 0.679 |
| Co1 | 4(f) | 1/3 | 2/3 | 0.61412(6) | 1 |
| Al1 | 4(e) | 0 | 0 | 0.1318(1) | 0.946 |
| Ga1 | 4(e) | 0 | 0 | 0.1318(1) | 0.054 |
| Al2 | 4(f) | 1/3 | 2/3 | 0.0455(1) | 1 |
| Si1 | 6(h) | 0.5367(5) | 0.073(1) | 1/4 | 0.322 |