Solidification simulations

We'll look at solidification in the Al-Zn system for an example Al-30Zn alloy.

In [1]:
```
import matplotlib.pyplot as plt
import numpy as np
from pycalphad import Database, binplot, variables as v
```

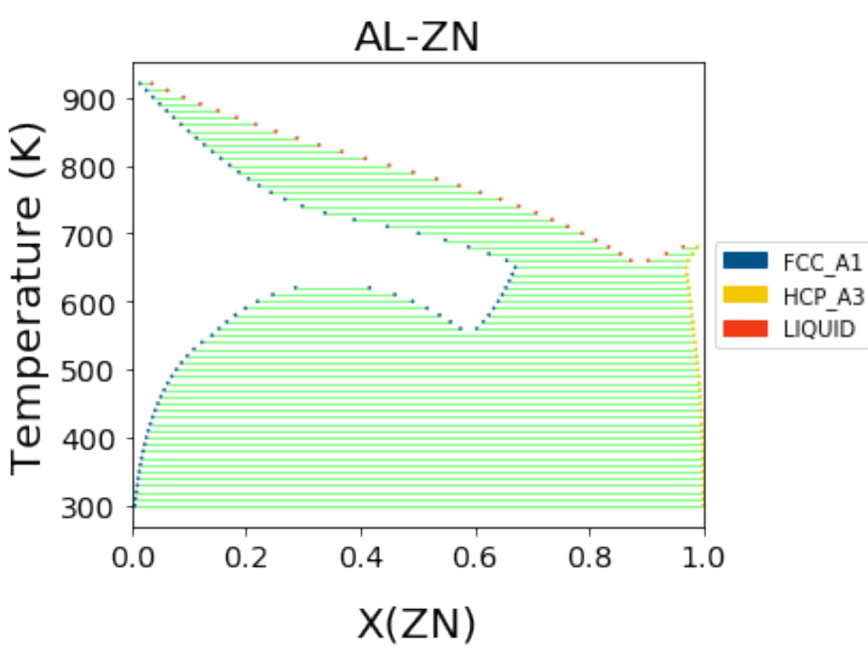
Load the database file for this system

In [2]:
```
dbf = Database('alzn_mey.tdb')
comps = ['AL', 'ZN', 'VA']
phases = sorted(dbf.phases.keys())
```

In [3]:
```
%%time
binplot(dbf, comps, phases, {v.P: 101325, v.N: 1, v.T: (300, 1000, 10)
, v.X('ZN'): (0, 1, 0.01)})
```

```
CPU times: user 14 s, sys: 173 ms, total: 14.1 s
Wall time: 14.1 s
```

Out[3]: <matplotlib.axes._subplots.AxesSubplot at 0x128de5978>



Equilibrium Solidification

Simulation

In [4]:
```
%%time

from scheil import simulate_equilibrium_solidification

initial_composition = {v.X('ZN'): 0.3}
start_temperature = 860

eq_sol_res = simulate_equilibrium_solidification(dbf, comps, phases, i
nitial_composition, start_temperature, step_temperature=1.0)
```

```
CPU times: user 4.85 s, sys: 192 ms, total: 5.04 s
Wall time: 5.1 s
```

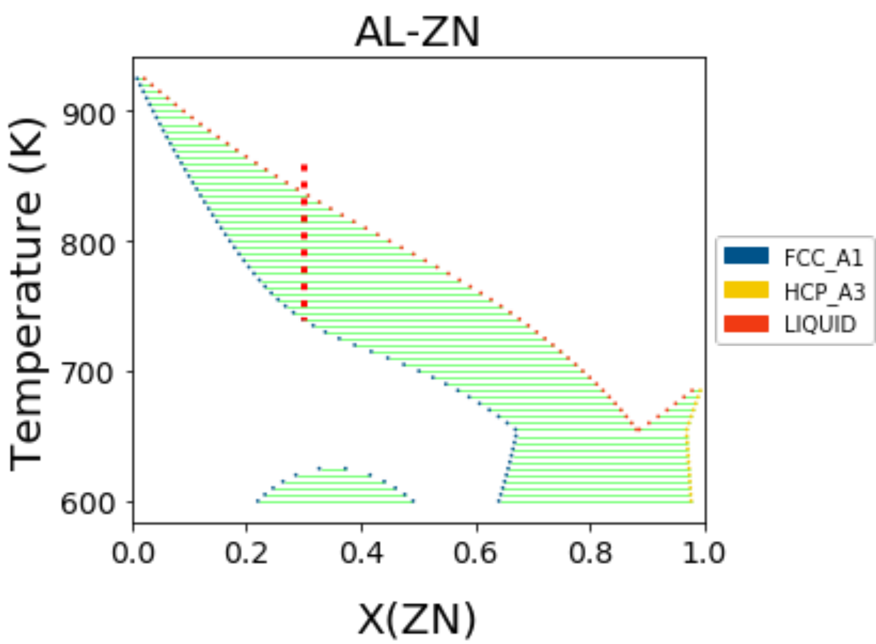
Solidification path

The solidification path follows the overall composition.

In [5]:
```
%%time
ax = binplot(dbf, comps, phases, {v.P: 101325, v.N: 1, v.T: (600, 1000
, 5), v.X('ZN'): (0, 1, 0.01)})
ax.plot(np.ones(len(eq_sol_res.temperatures))*0.3, eq_sol_res.temperat
ures, linestyle=':', color='red', lw=3)
```

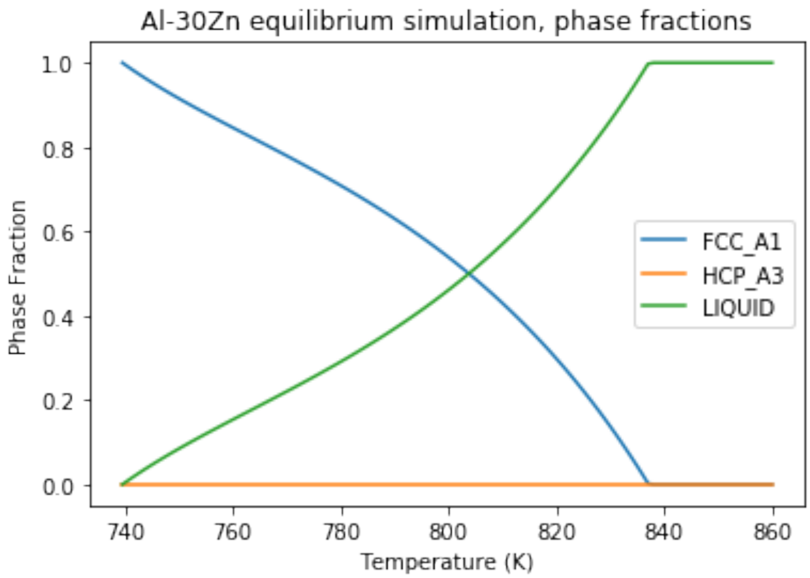
```
CPU times: user 17 s, sys: 127 ms, total: 17.1 s
Wall time: 17.1 s
```

Out[5]: [<matplotlib.lines.Line2D at 0x128de57b8>]



Phase fractions

In [6]:
```
for phase_name, amounts in eq_sol_res.cum_phase_amounts.items():
    plt.plot(eq_sol_res.temperatures, amounts, label=phase_name)
plt.plot(eq_sol_res.temperatures, eq_sol_res.fraction_liquid, label='L
IQUID')
plt.ylabel('Phase Fraction')
plt.xlabel('Temperature (K)')
plt.title('Al-30Zn equilibrium simulation, phase fractions')
plt.legend(loc='best')
plt.show()
```



Scheil solidification

In [7]:
```
%%time

from scheil import simulate_scheil_solidification

initial_composition = {v.X('ZN'): 0.3}
start_temperature = 860

sol_res = simulate_scheil_solidification(dbf, comps, phases, initial_c
omposition, start_temperature, step_temperature=1.0)
```

```
CPU times: user 14.6 s, sys: 462 ms, total: 15.1 s
Wall time: 15.1 s
```

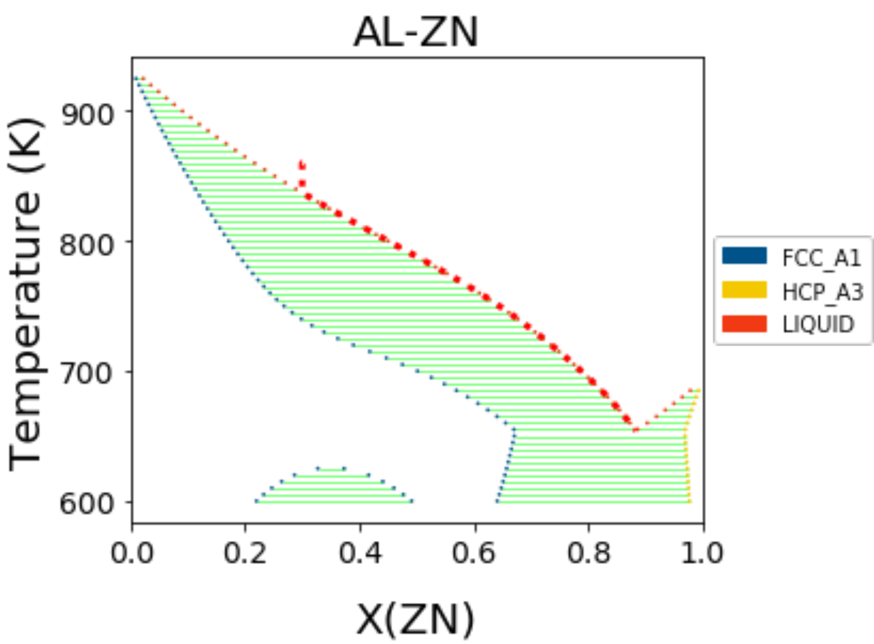
Solidification path

In Scheil solidification, the solidification path follows the liquidus composition, since the liquid has perfect mixing and is in local equilibrium with the solid at each temperature.

In [8]:
```
%%time
ax = binplot(dbf, comps, phases, {v.P: 101325, v.N: 1, v.T: (600, 1000
, 5), v.X('ZN'): (0, 1, 0.01)})
ax.plot(sol_res.x_liquid['ZN'], sol_res.temperatures, linestyle=':', c
olor='red', lw=3)
```

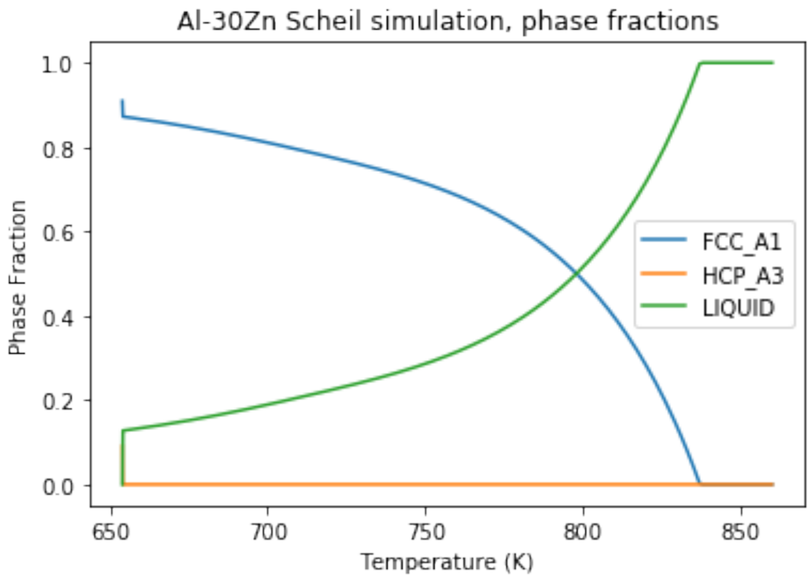
```
CPU times: user 17.4 s, sys: 125 ms, total: 17.6 s
Wall time: 17.6 s
```

Out[8]:
```
[<matplotlib.lines.Line2D at 0x12babc5c0>]
```

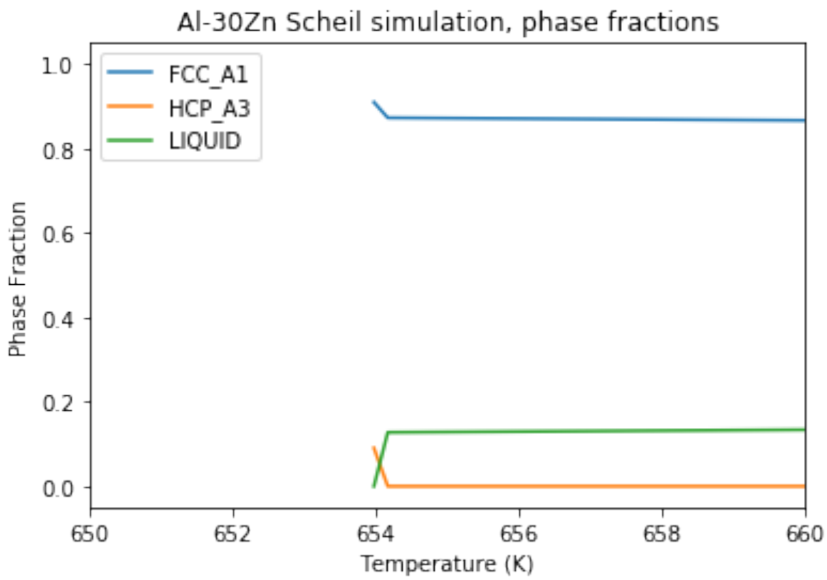


Phase fractions

In [9]:
```
for phase_name, amounts in sol_res.cum_phase_amounts.items():
    plt.plot(sol_res.temperatures, amounts, label=phase_name)
plt.plot(sol_res.temperatures, sol_res.fraction_liquid, label='LIQUID'
)
plt.ylabel('Phase Fraction')
plt.xlabel('Temperature (K)')
plt.title('Al-30Zn Scheil simulation, phase fractions')
plt.legend(loc='best')
plt.show()
```



In [10]:
```
for phase_name, amounts in sol_res.cum_phase_amounts.items():
    plt.plot(sol_res.temperatures, amounts, label=phase_name)
plt.plot(sol_res.temperatures, sol_res.fraction_liquid, label='LIQUID'
)
plt.ylabel('Phase Fraction')
plt.xlabel('Temperature (K)')
plt.title('Al-30Zn Scheil simulation, phase fractions')
plt.legend(loc='best')
plt.xlim(650, 660)
plt.show()
```



In [ ]: