# Constraints A:

C1: Al < Ti

C2: 3 < FCC < 10

## Case 1: C1 & C2: Al < Ti, 3 < FCC < 10

==========Single objective optimization=========

The minimum objective function value is: 1000.0641926745976

Optimized composition:

Ni = 16.89371060393026wt%

Ti = 4.224127275611192wt%

Al = 2.5772248072333843wt%

wt% Ni3Ti = [18.75600542]

wt% Laves = [0.]

wt% FCC = [3.12652513]

Ni3Ti formation temperature = [806.752]

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## Case 2: relax C1: Allow Al > Ti, 3 < FCC < 10

==========Single objective optimization=========

The minimum objective function value is: 999.7947574711959

Optimized composition:

Ni = 19.847338142267827wt%

Ti = 4.984675105525493wt%

Al = 6.9277648243625025wt%

wt% Ni3Ti = [22.17289431]

wt% Laves = [0.09079716]

wt% FCC = [3.30000066]

Ni3Ti formation temperature = [670.54]

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## Case 3: relax C2: Al < Ti, 3 < FCC (no upper limit)

==========Single objective optimization=========

The minimum objective function value is: 0.06349291242434663

Optimized composition:

Ni = 16.740085482652034wt%

Ti = 4.430889088463662wt%

Al = 2.6498605810325997wt%

wt% Ni3Ti = [18.70613895]

wt% Laves = [0.]

wt% FCC = [3.12390423]

Ni3Ti formation temperature = [804.078]

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## Case 4: relax both C1 and C2: allow Al > Ti, 3 < FCC (no upper limit):

==========Single objective optimization=========

The minimum objective function value is: -0.20502507101097134

Optimized composition:

Ni = 19.64104776919373wt%

Ti = 4.607058638503721wt%

Al = 6.66371770048884wt%

wt% Ni3Ti = [22.21736266]

wt% Laves = [0.08142067]

wt% FCC = [3.62644239]

Ni3Ti formation temperature = [672.73]

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## Observations:

1. Case 1 & 3 have the same result, Case 2 & 4 also have the same result. So the upper limit of FCC has no effect on the result (when FCC>3). FCC will be minimized (although not included in the objective function) in order to maximize Ni3Ti. Refer to the correlation matrix for the inverse correlation (-0.898) between FCC and Ni3Ti
2. If Al > Ti is allowed, Case 2 & 4 have lower T\_Ni3Ti and more wt% Ni3Ti than Case 1 & 3, but slightly more Laves. From the correlation matrix, Al and Ni3Ti have negative correlation (-0.682), Al and T\_Ni3Ti also have negative correlation (-0.476), Al and Laves have positive but not small correlation (0.119)

# Constraints B:

C1: Al < Ti

C2: 9 < FCC

## Case 1: C1 & C2: Al < Ti, 9 < FCC

==========Single objective optimization=========

The minimum objective function value is: 0.327617647492502

Optimized composition:

Ni = 16.669083955278033wt%

Ti = 3.1388036689182117wt%

Al = 2.139553108476724wt%

wt% Ni3Ti = [14.03196682]

wt% Laves = [0.]

wt% FCC = [9.02098204]

Ni3Ti formation temperature = [883.15]

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## Case 2: relax C1: allow Al > Ti, 9 < FCC

==========Single objective optimization=========

The minimum objective function value is: 0.007137305891338042

Optimized composition:

Ni = 19.56234995479491wt%

Ti = 4.352200918359936wt%

Al = 8.592912888940086wt%

wt% Ni3Ti = [12.02149437]

wt% Laves = [0.25995806]

wt% FCC = [13.85699417]

Ni3Ti formation temperature = [477.19598245]

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## Observation:

1. If Al > Ti is allowed, T\_Ni3Ti decreases significantly, and wt% Ni3Ti decreases only slightly.