# ML Final Project

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日期：2021 / 06 / 15

# Outline

1. Introduction
2. Training database
3. ANN model
4. Validation result
5. Solve
6. Result and discussion

# *Introduction*

1. ML application on high entropy alloy lattice distortion effect
2. Ternary alloy system : **FeCrNi**
3. Compare **delta** and **average atomic shear strain(AASS)**

**Delta** → $\delta = 100\sqrt{\sum_{i=1}^{n} c_i(1 - r_i/\bar{r})^2}$

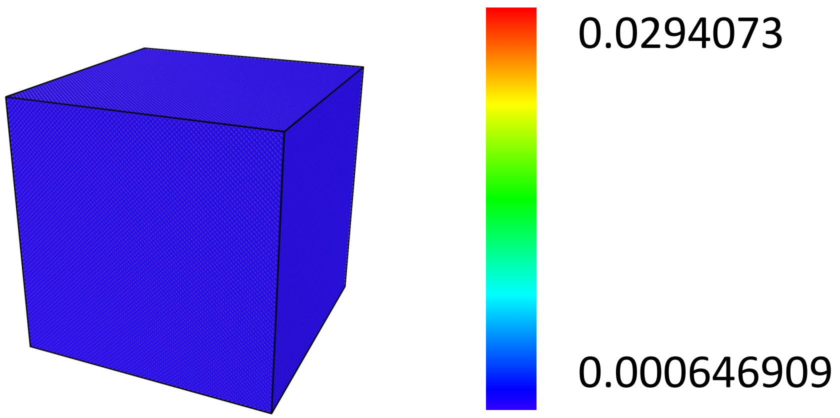
**AASS** → MD simulation

4. The prediction of AASS from machine learning can apply on dislocation behavior research

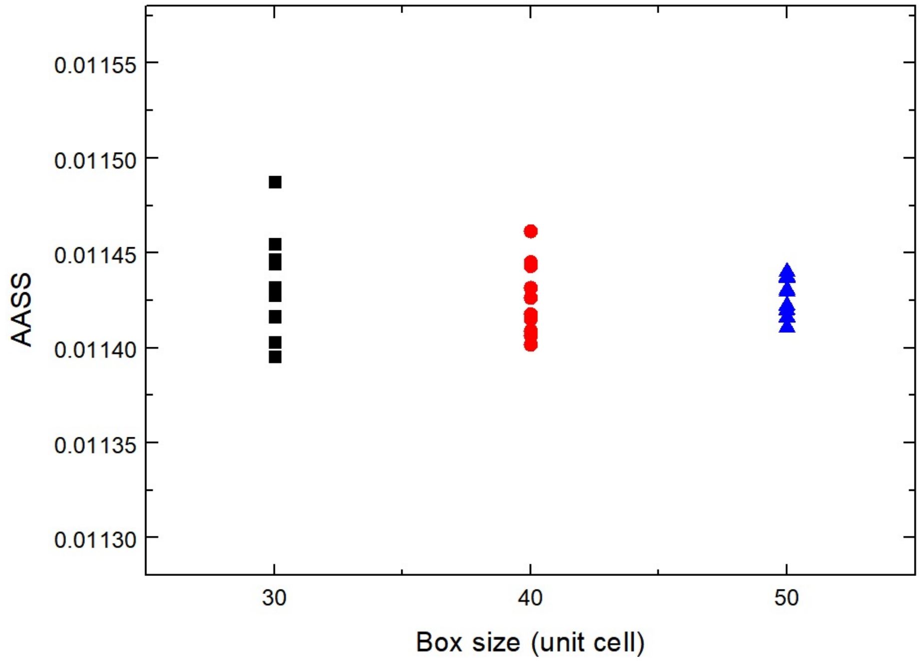
# *Introduction*

1. Box size 50×50×50 (unit cell)
2. 500000 atoms
3. $Fe_{33.3}Cr_{33.3}Ni_{33.3}$
4. Equiatomic alloy
5. Temperature = 0K
6. Cg minimization
7. Average atomic shear strain

$$(\eta_{\text{ave}}) = \frac{\sum_{i=1}^{500000} \eta_i}{500000}$$




Random seed and box size test result



# Introduction

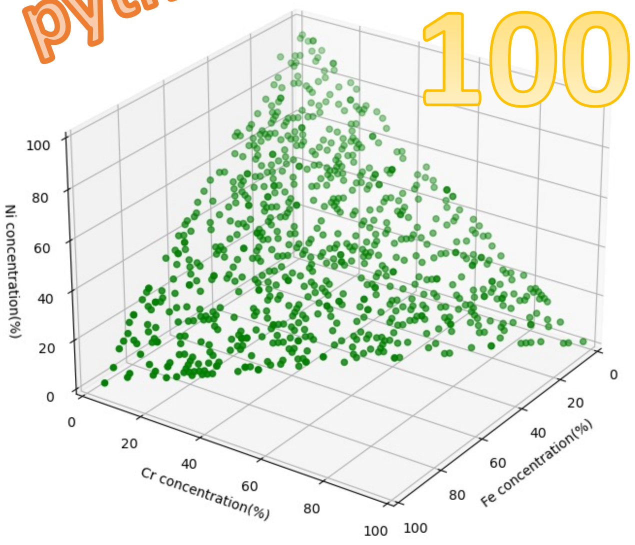
＊ $Fe_xCr_yNi_z$ 此合金共有 4851 種不同的成分組成

| Fe (%) | Cr (%) | Ni (%) |
|---|---|---|
| 1 | 1 | 98 |
| 1 | 2 | 97 |
| 1 | 3 | 96 |
| 1 | 4 | 95 |
| 1 | 5 | 94 |
| 1 | 6 | 93 |
| 1 | 7 | 92 |
| 1 | 8 | 91 |
| 1 | 9 | 90 |
| 1 | 10 | 89 |
| 1 | 11 | 88 |
| ⋮ | ⋮ | ⋮ |
| 97 | 2 | 1 |
| 98 | 1 | 1 |

4851

python

1000




X+Y+Z=100

input

Delta(formula)

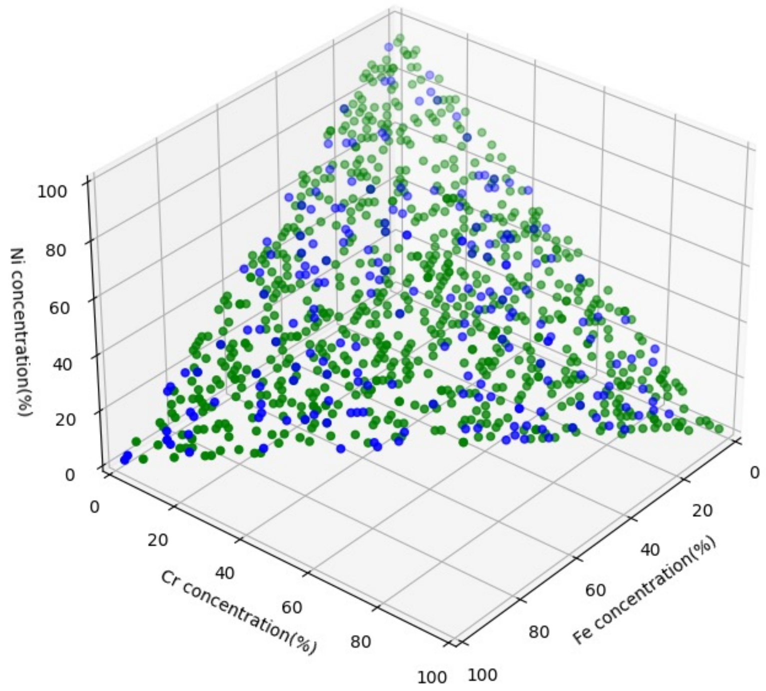
AASS(MD)

output

# Training database

X+Y+Z=100

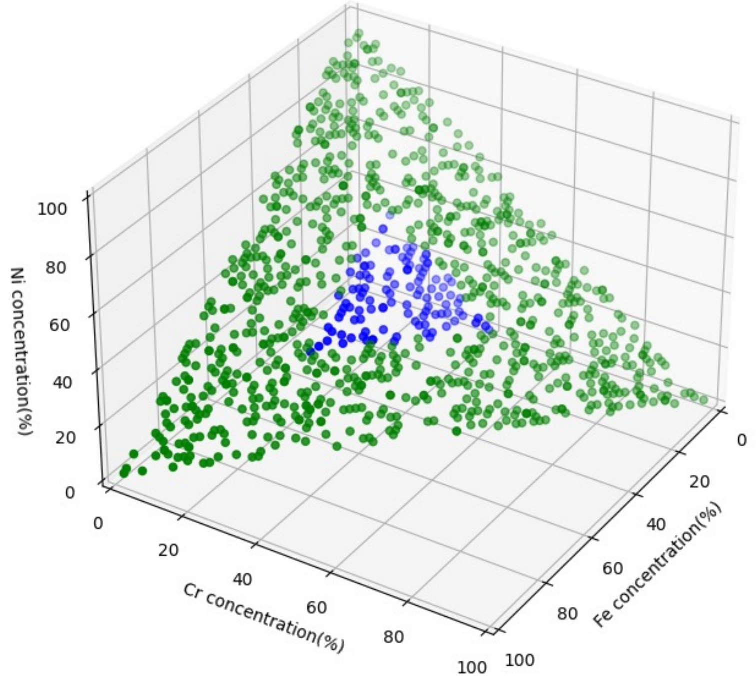
1000




Train : 700
Test : 100
Validation : 200

800

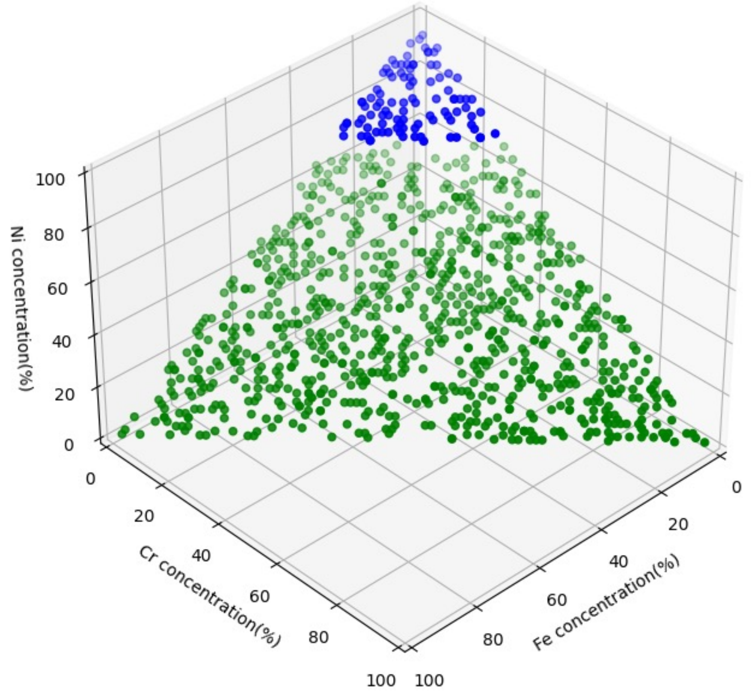
1000




Train : 700
Test : 186
Validation :114

886

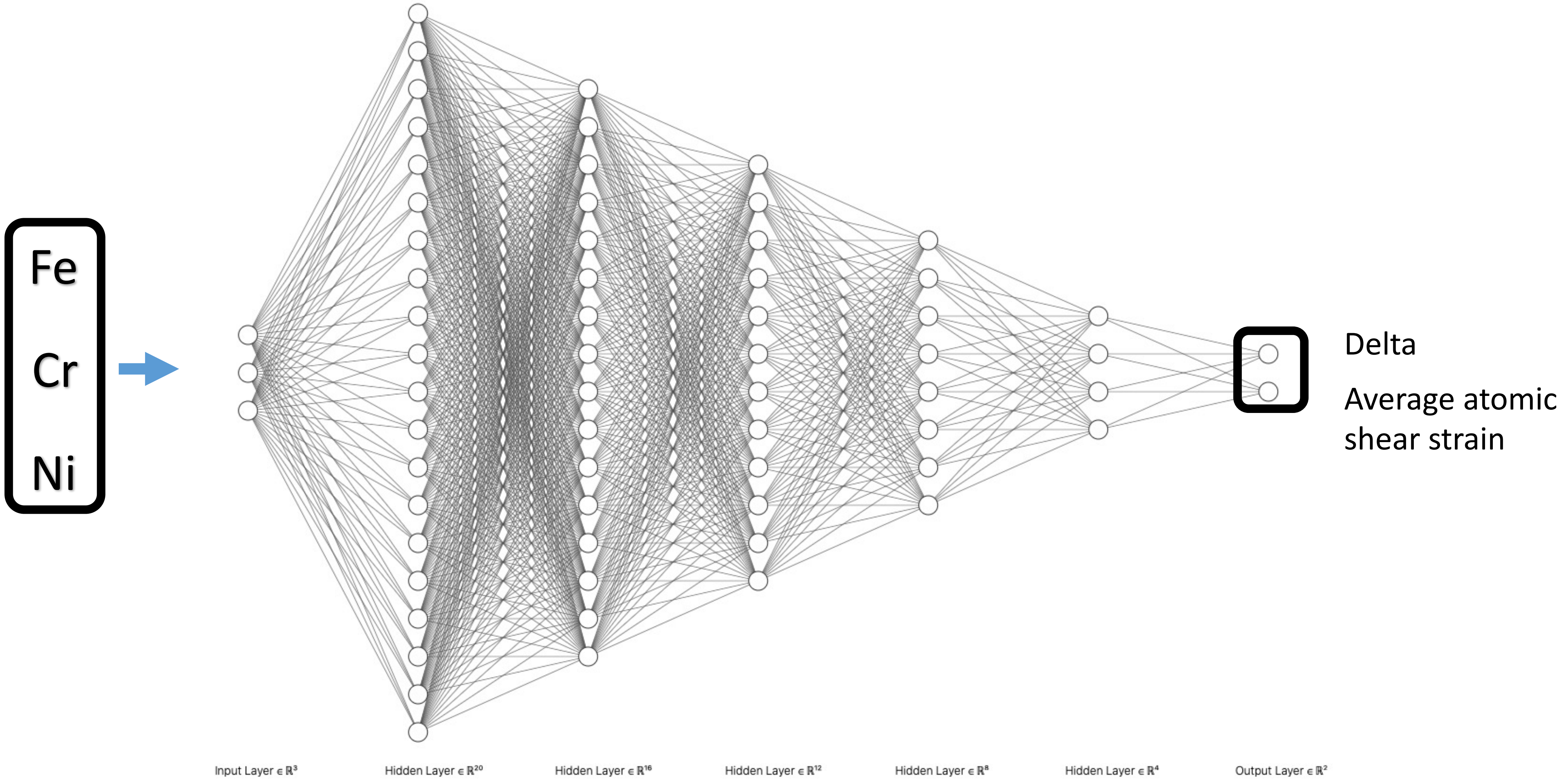
1000




Train : 700
Test : 203
Validation : 97

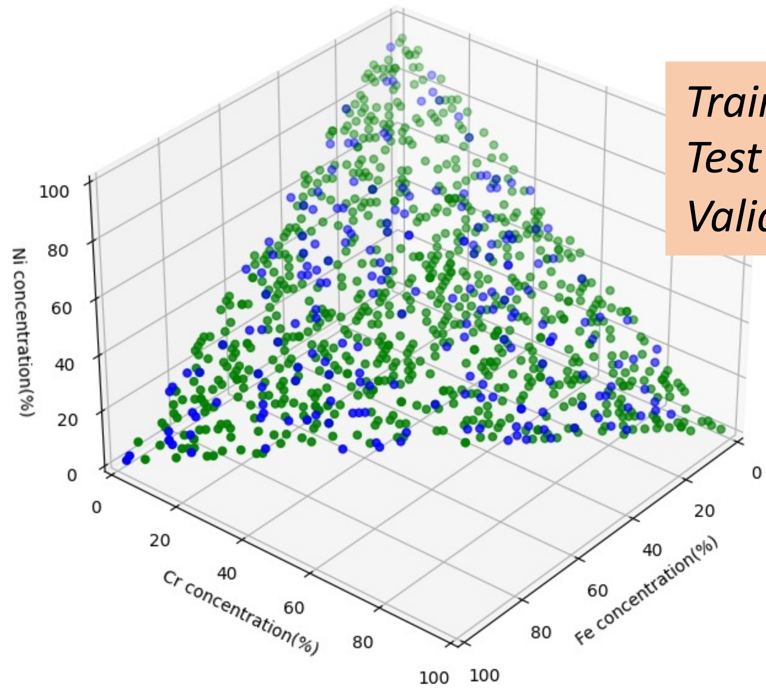
903

# ANN model



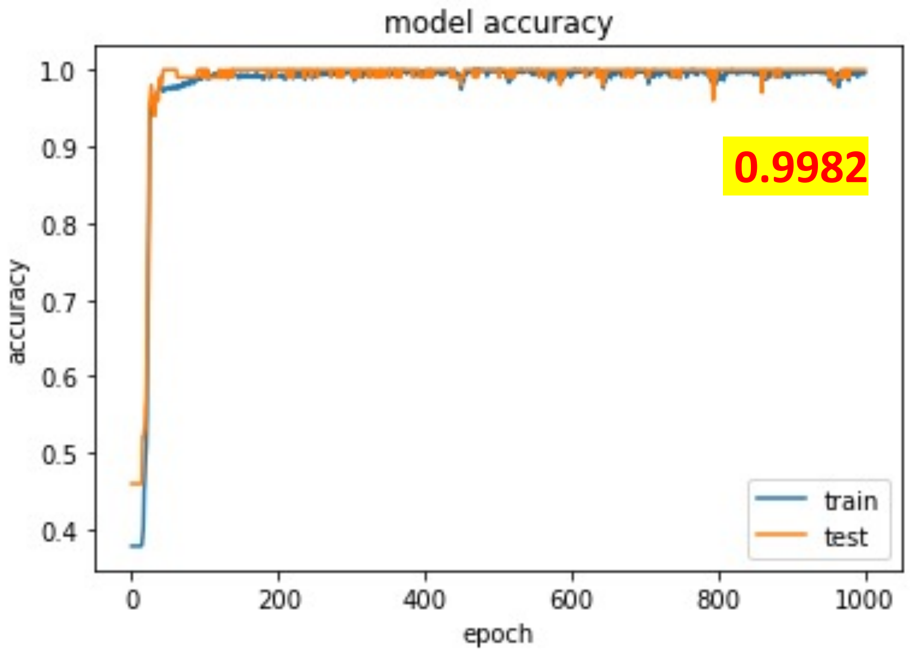
Fe
Cr
Ni
Delta
Average atomic shear strain
Input Layer ∈ ℝ³
Hidden Layer ∈ ℝ²⁰
Hidden Layer ∈ ℝ¹⁶
Hidden Layer ∈ ℝ¹²
Hidden Layer ∈ ℝ⁸
Hidden Layer ∈ ℝ⁴
Output Layer ∈ ℝ²

# *Validation result1*

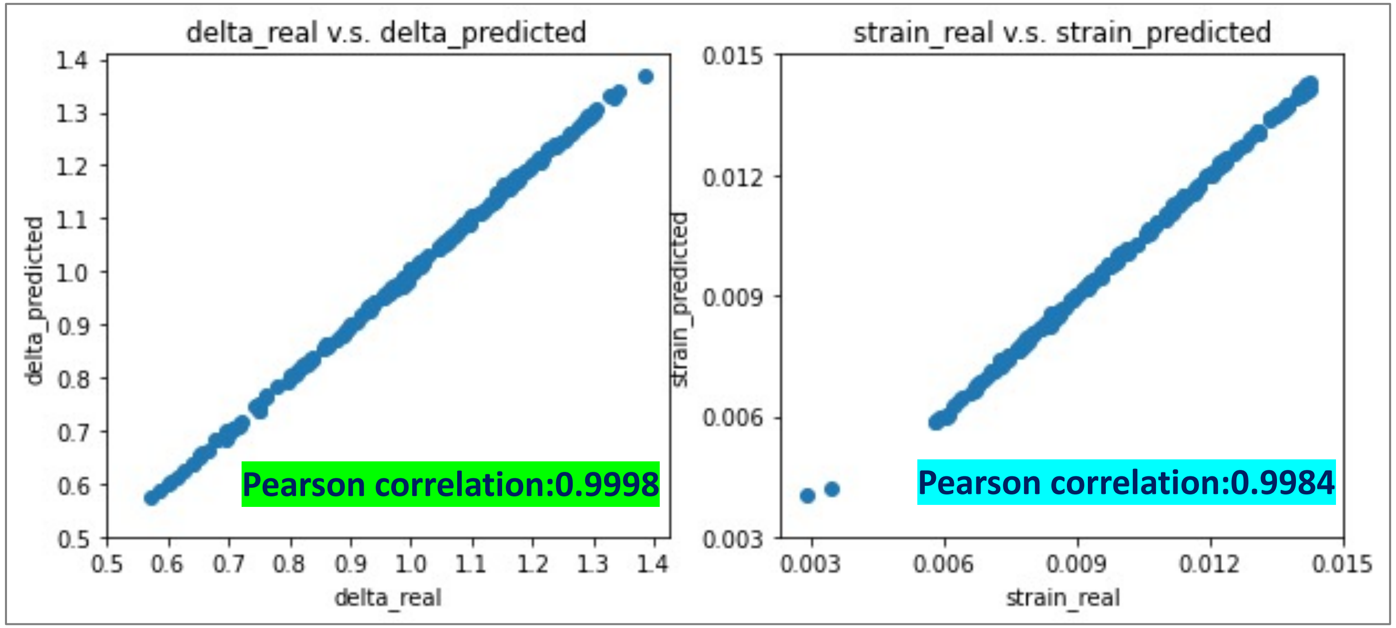



*Train : 700*
*Test : 100*
*Validation : 200*

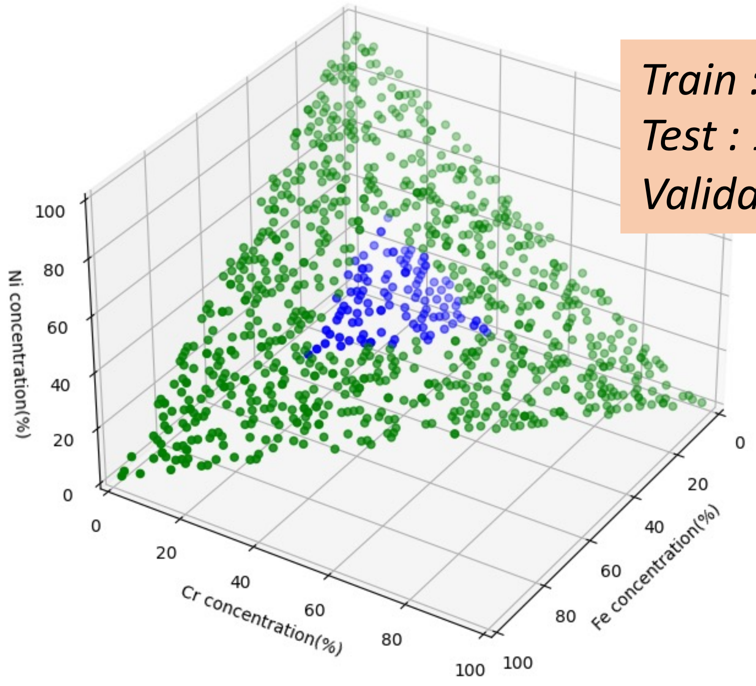
800




**Hidden layers : 6**
**Nodes : (128, 64, 64, 32, 16, 8)**
**Epochs : 800**
**Learning rate : 0.001**
**Activation function : Relu**

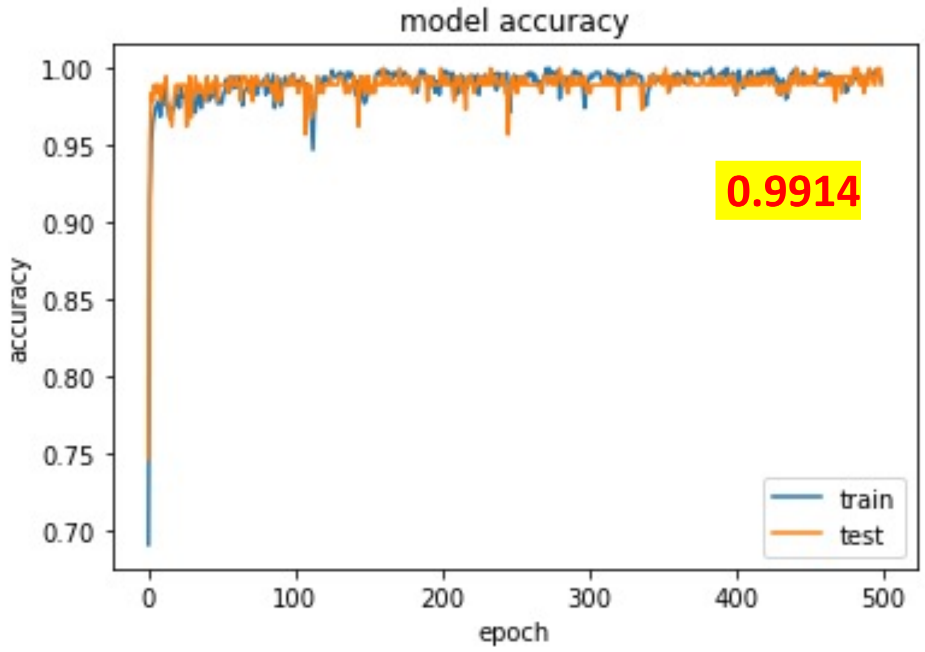


# *Validation result2*

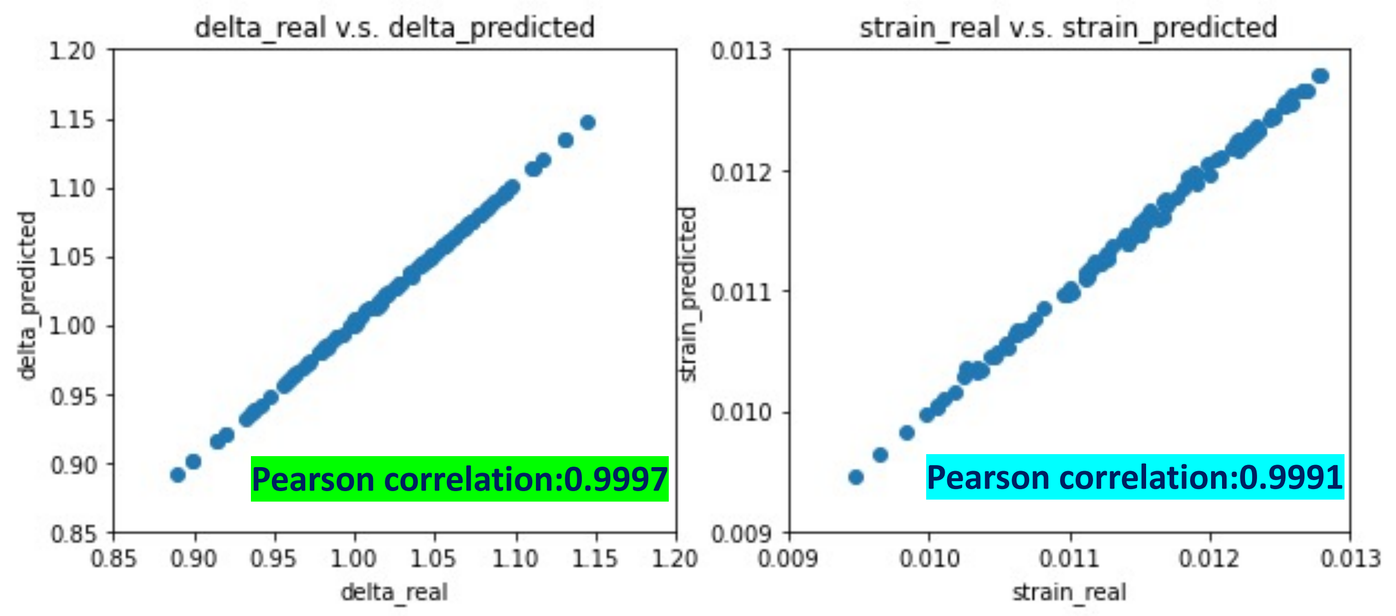



*Train : 700*
*Test : 186*
*Validation : 114*

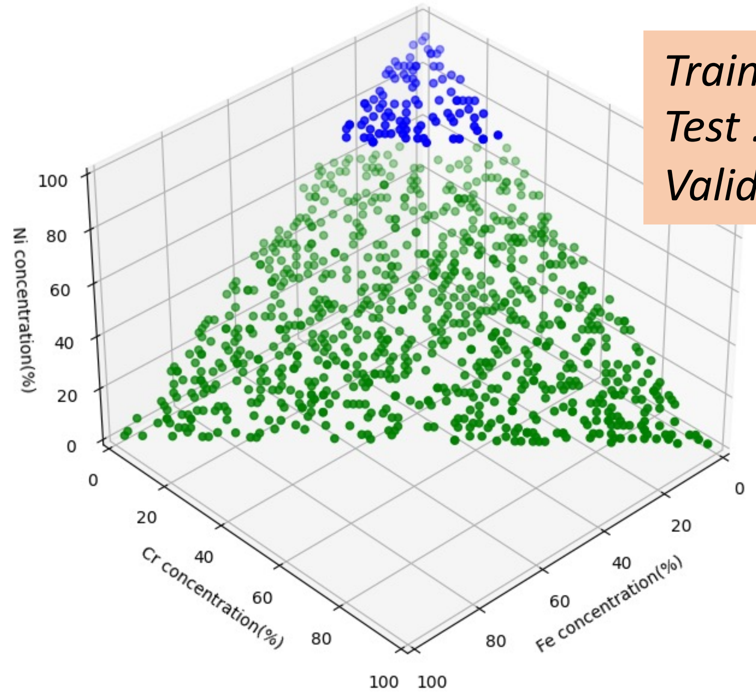
886



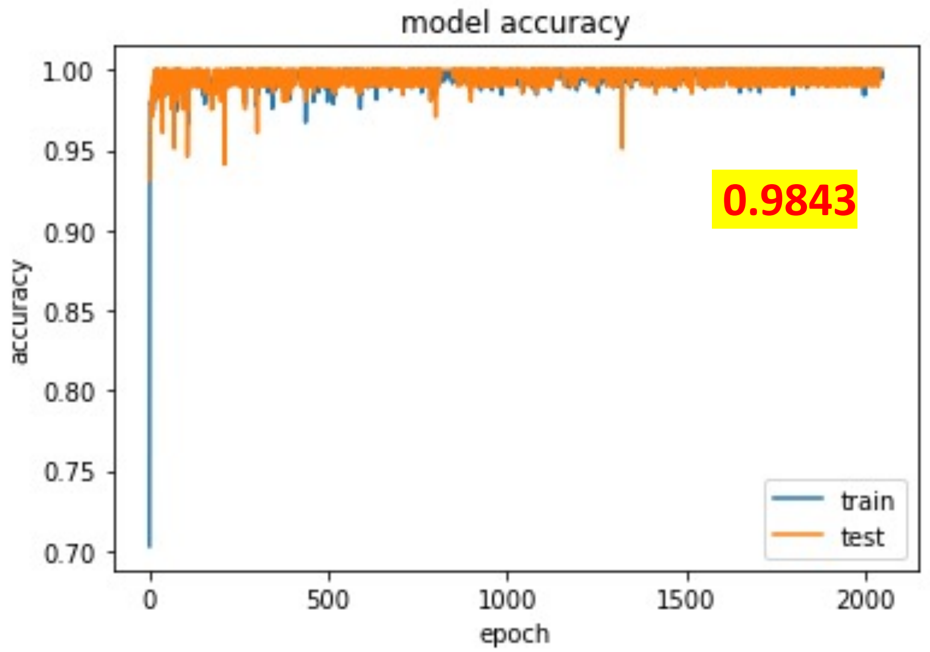

**Hidden layers : 7**
**Nodes : (512, 256, 128, 64, 32, 16, 8)**
**Epochs : 500**
**Learning rate : 0.001**
**Activation function : Relu**

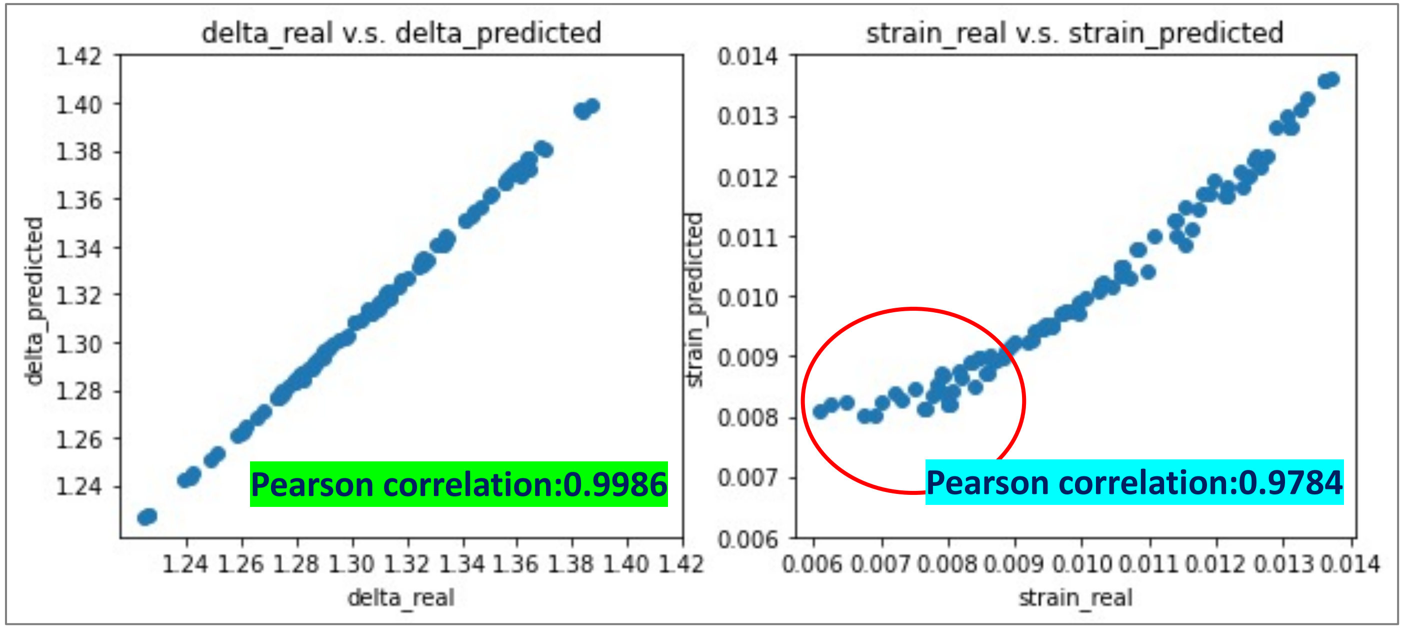


# *Validation result3*




*Train : 700*
*Test : 203*
*Validation : 97*
903

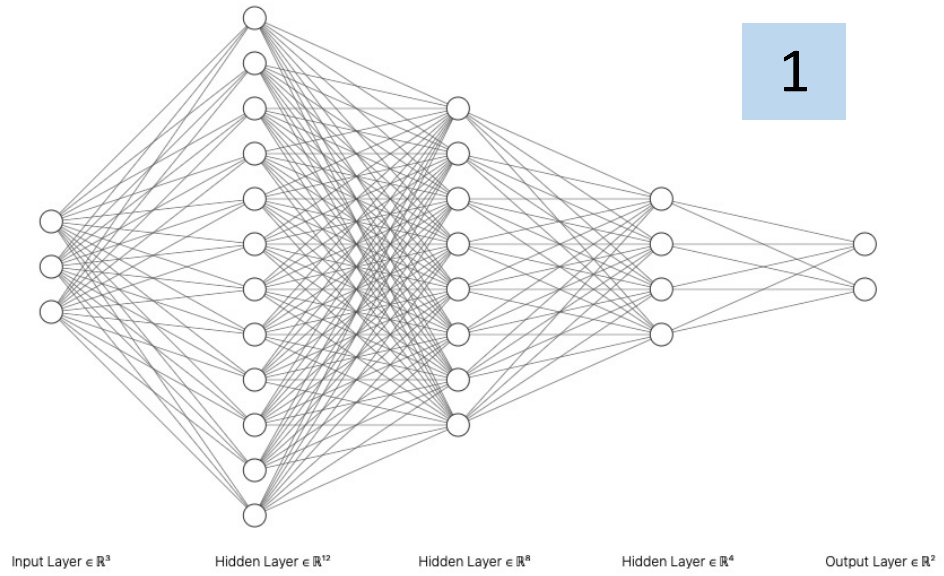


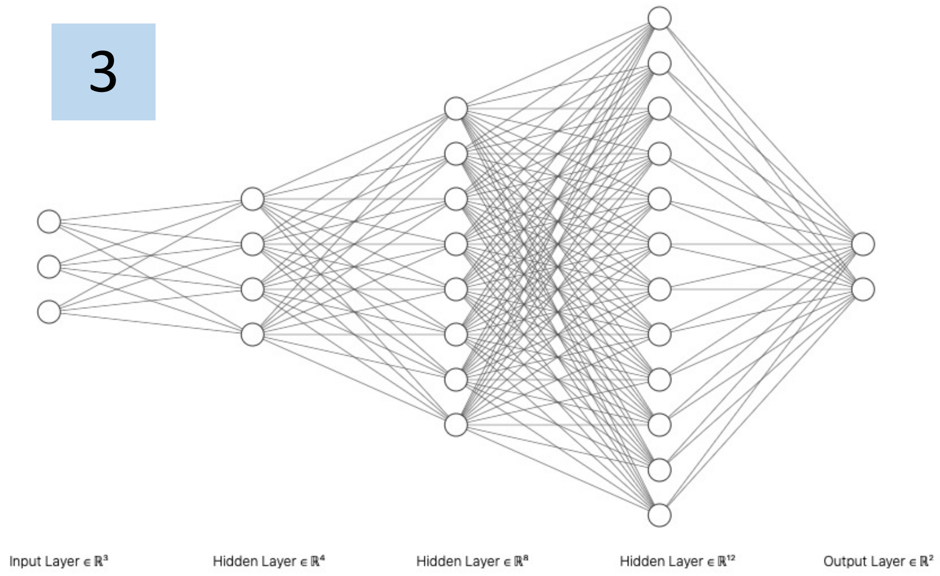

**Hidden layers : 8**
**Nodes : (512, 256, 128, 64, 32, 16, 8, 4)**
**Epochs : 2048**
**Learning rate : 0.001**
**Activation function : Relu**

# Solve – ANN model

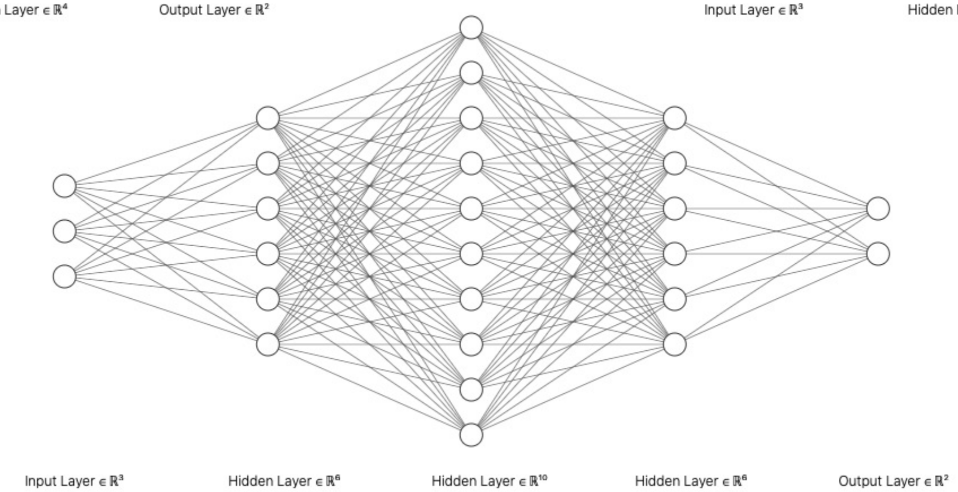
1




3

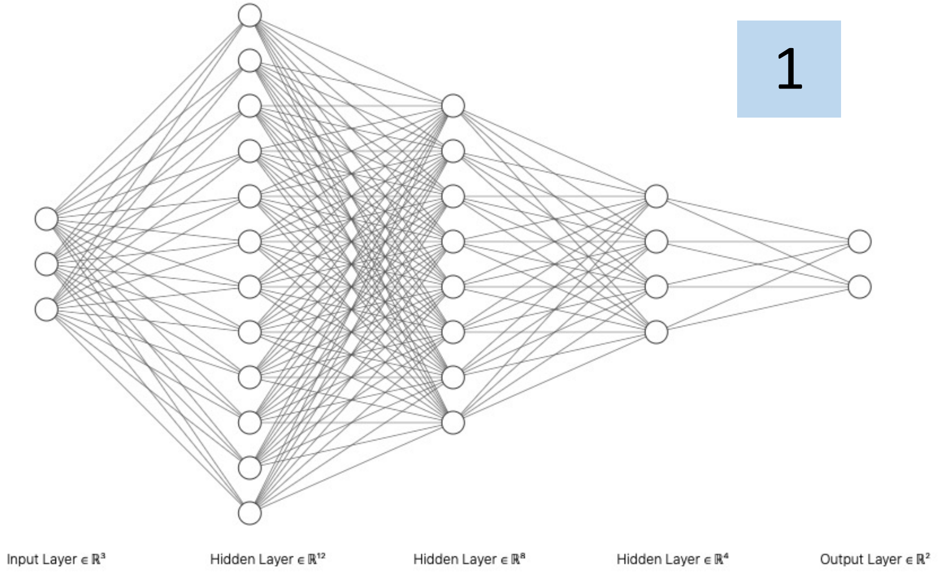



2

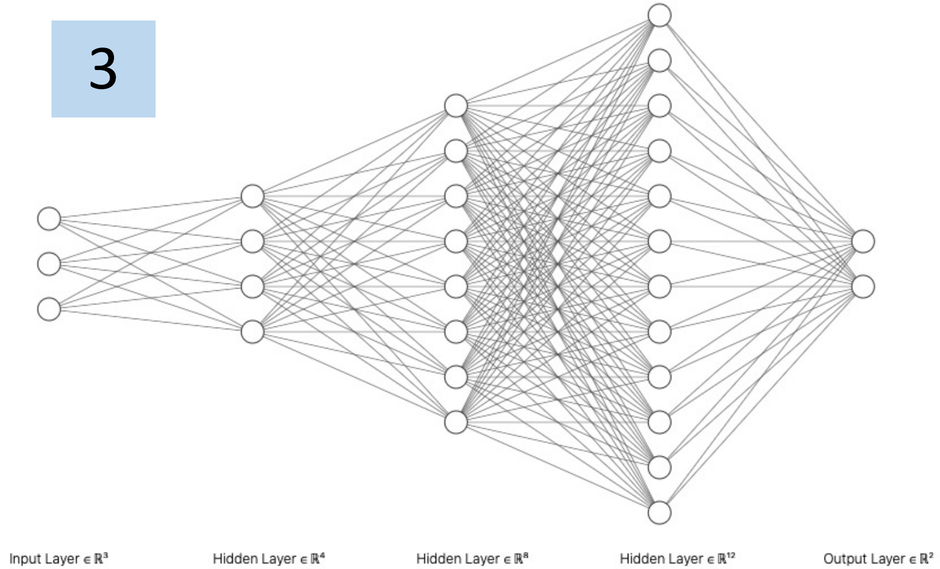


# Solve – ANN model

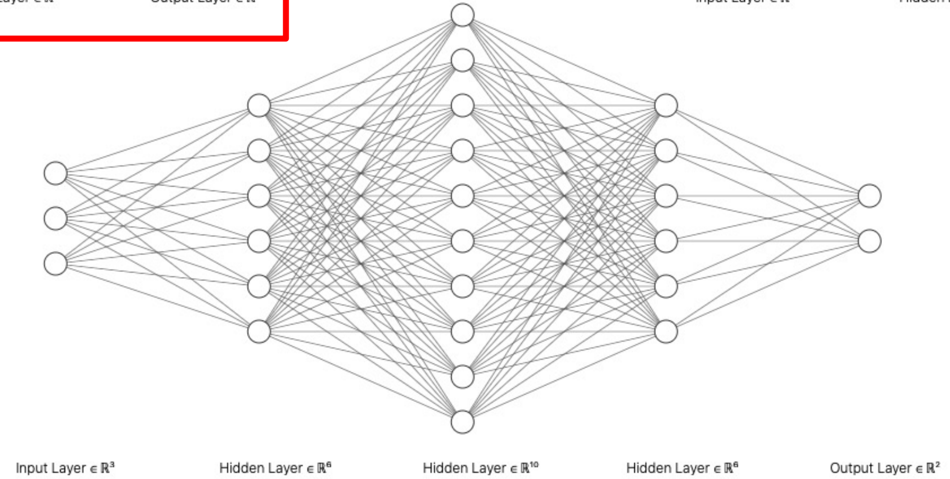
1




3

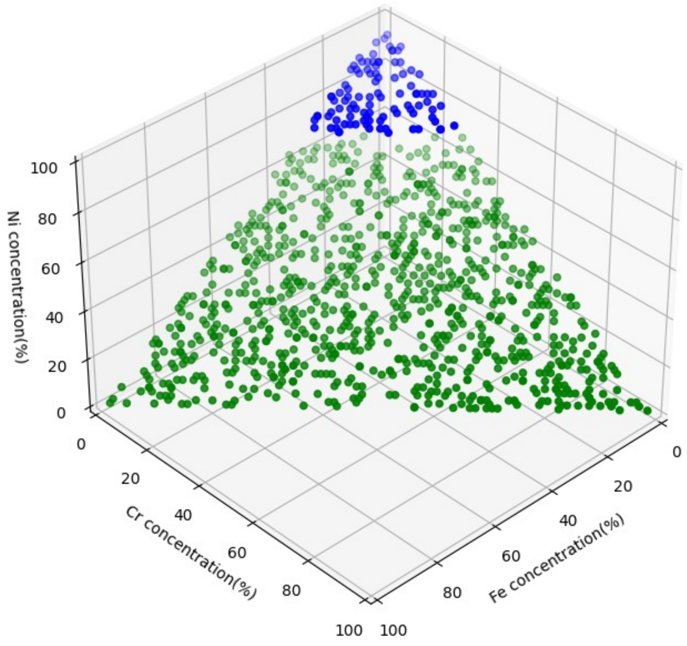



2



# Solve – training database (add)

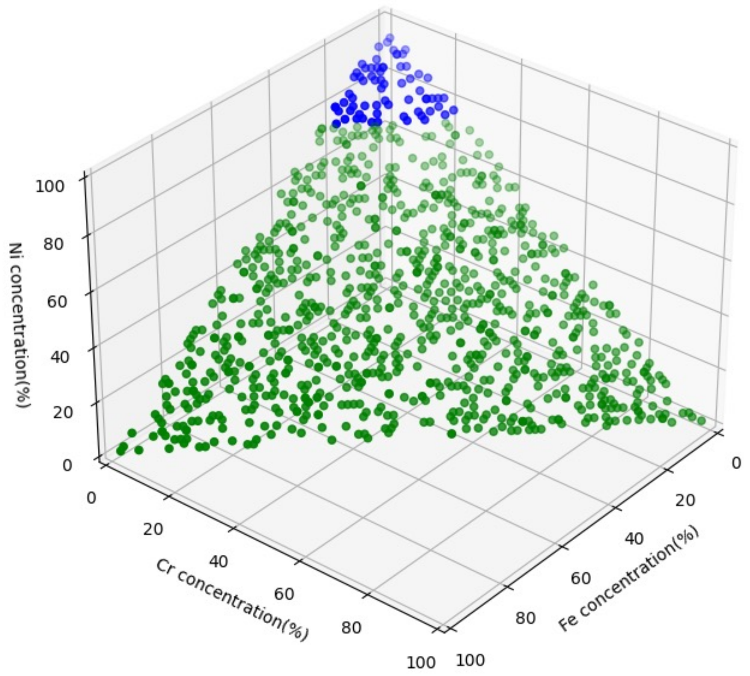
**Cr, Fe ≤ 30**
**Ni ≥ 70**




Train : 700
Test : 203
Validation : 97

903

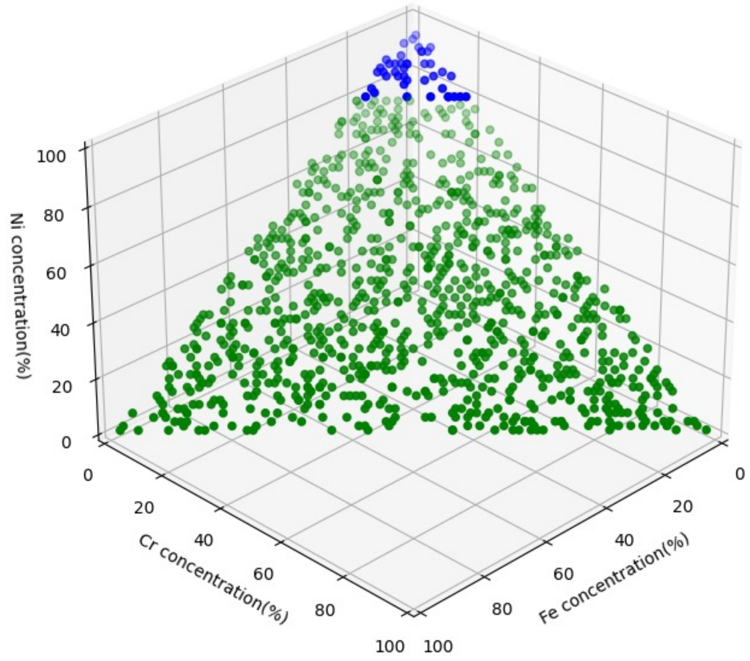
**Cr, Fe ≤ 25**
**Ni ≥ 75**




Train : 700
Test : 234
Validation : 66

934

**Cr, Fe ≤ 20**
**Ni ≥ 80**

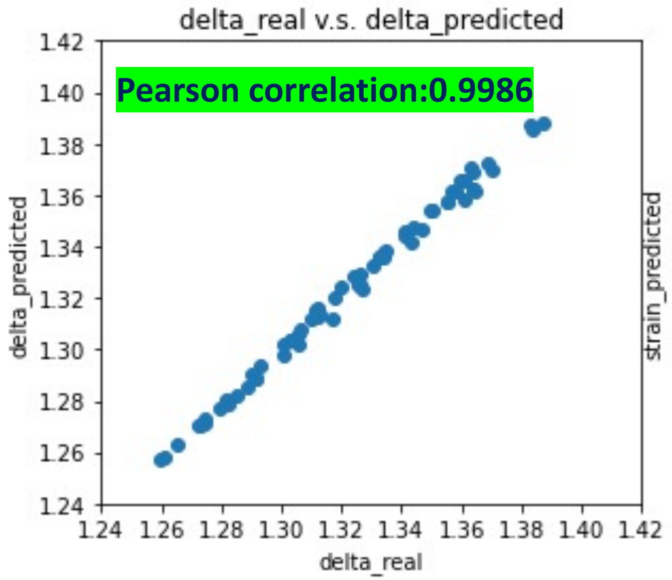


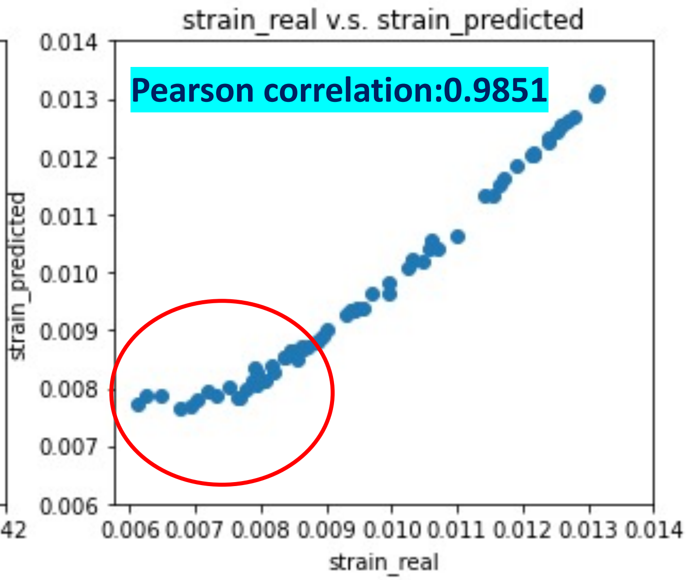

Train : 700
Test : 259
Validation : 41

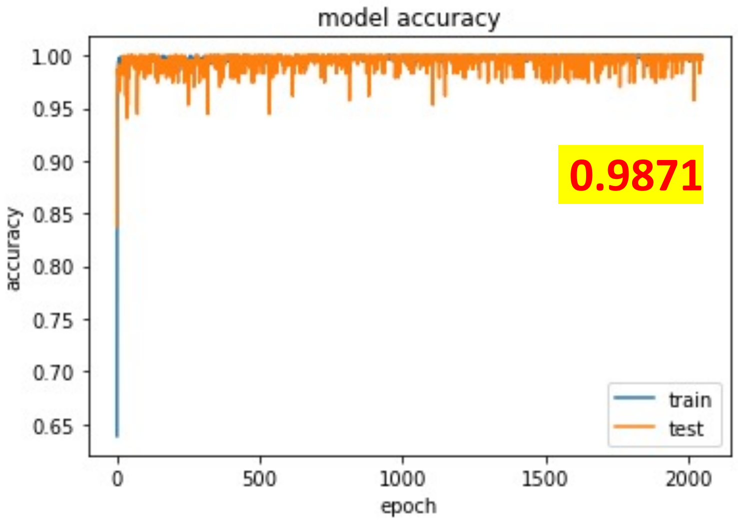
959

# ***Solve – validation result***

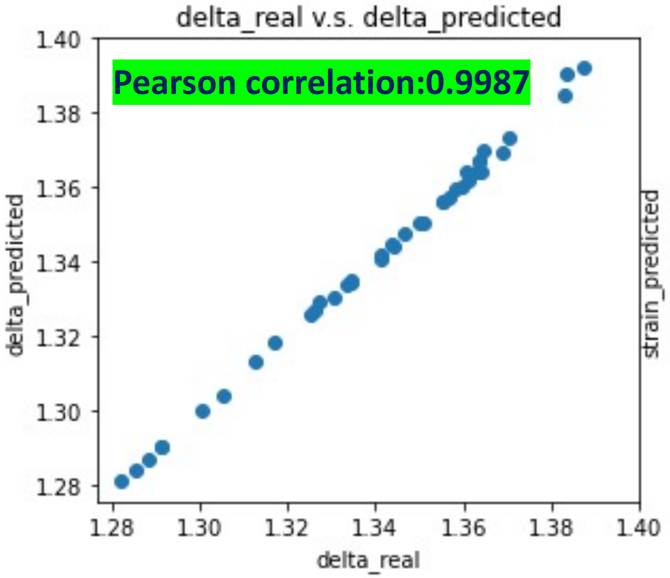
***Cr, Fe ≤ 25***
***Ni ≥ 75***

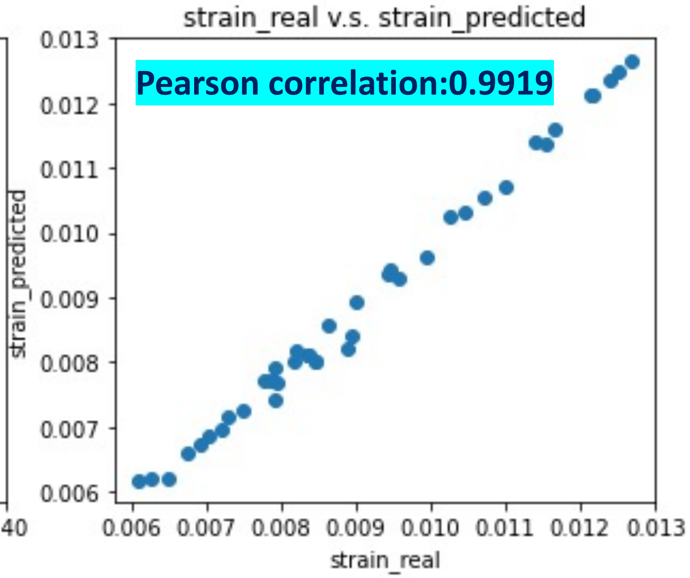


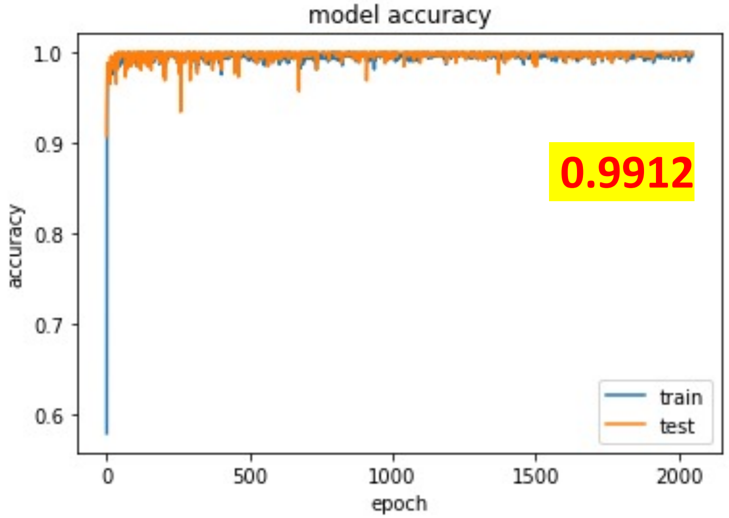




***Cr, Fe ≤ 20***
***Ni ≥ 80***

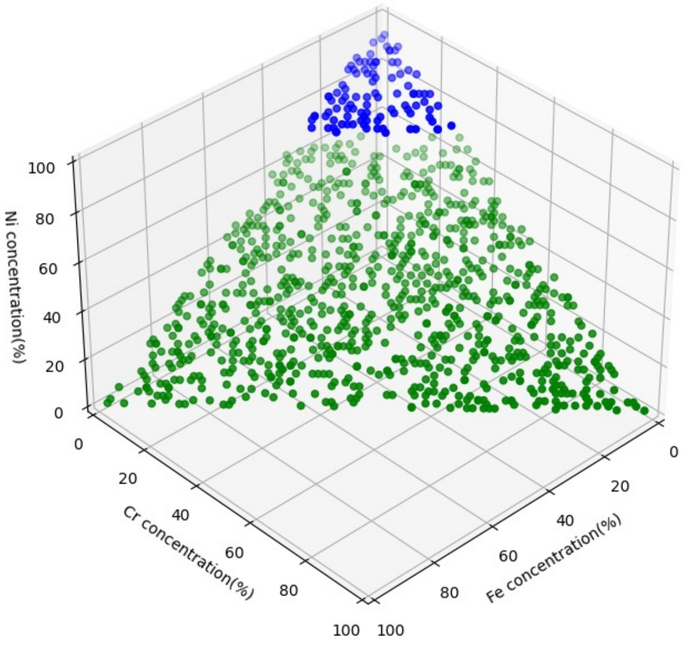


# Solve – training database (add)

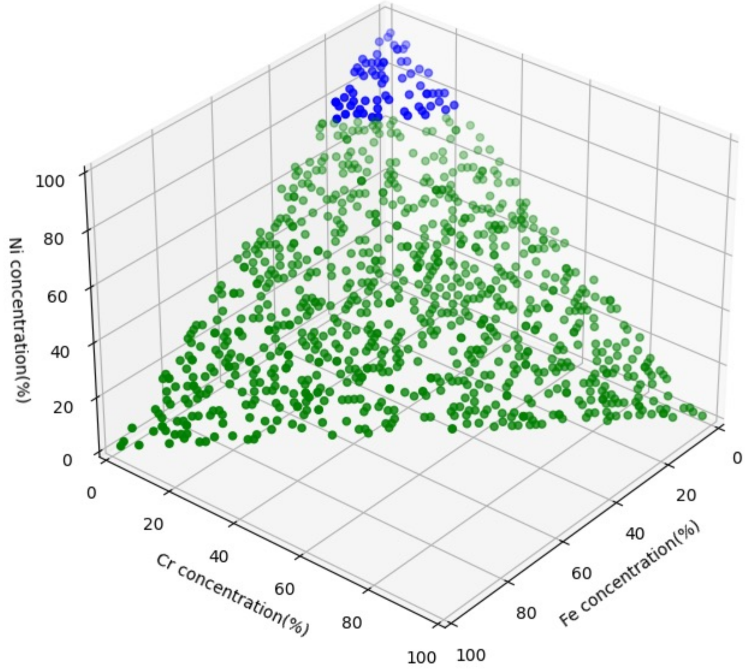
**Cr, Fe ≤ 30**
**Ni ≥ 70**




Train : 700
Test : 203
Validation : 97

903

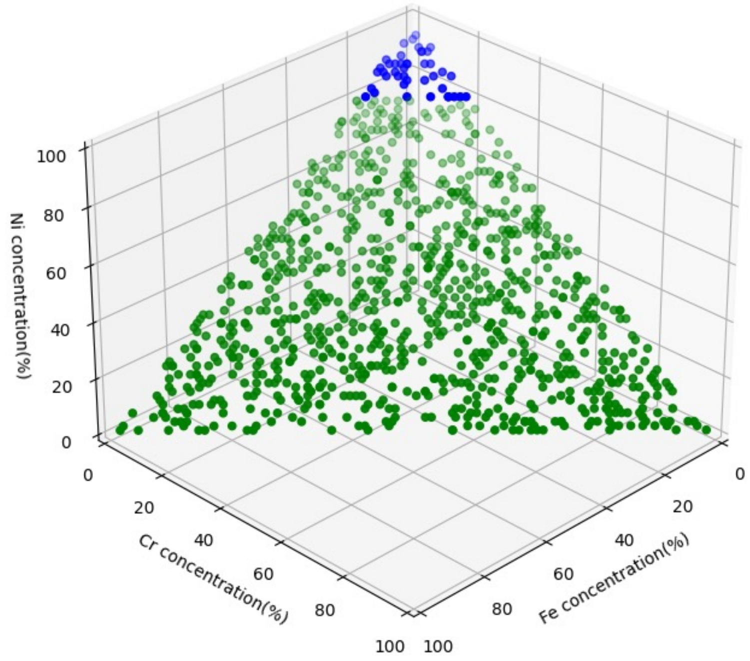
**Cr, Fe ≤ 25**
**Ni ≥ 75**




Train : 700
Test : 234
Validation : 66

934

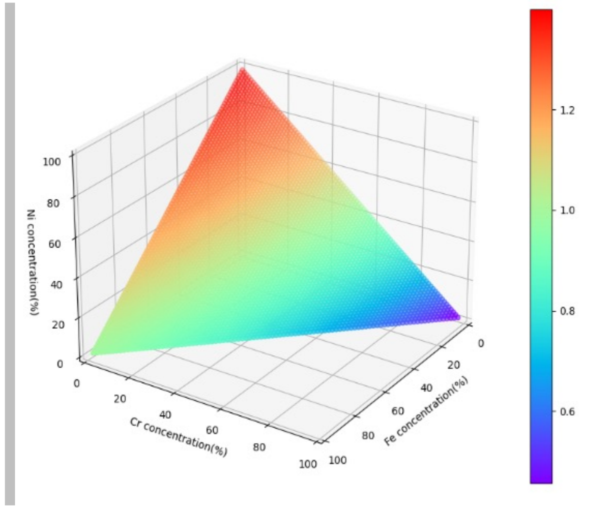
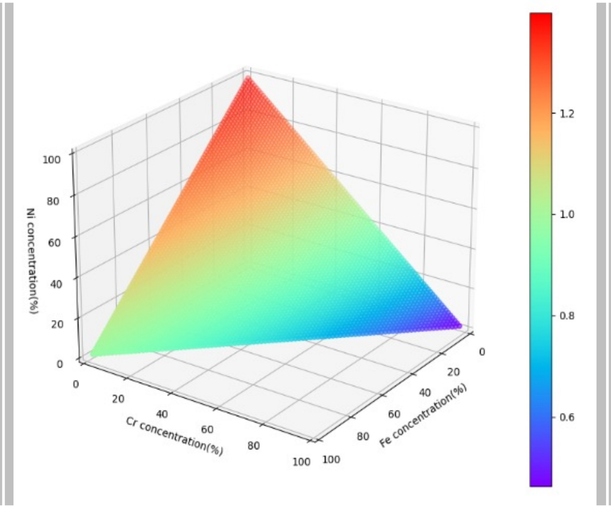
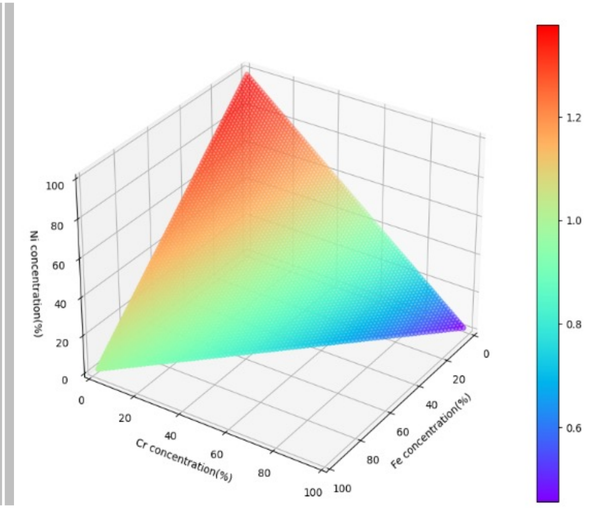
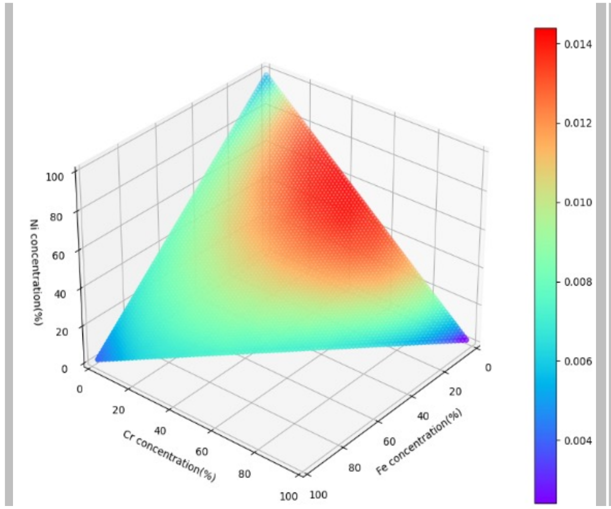
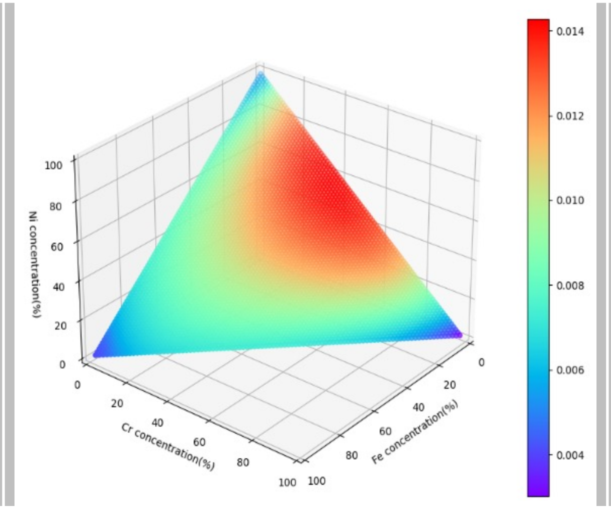
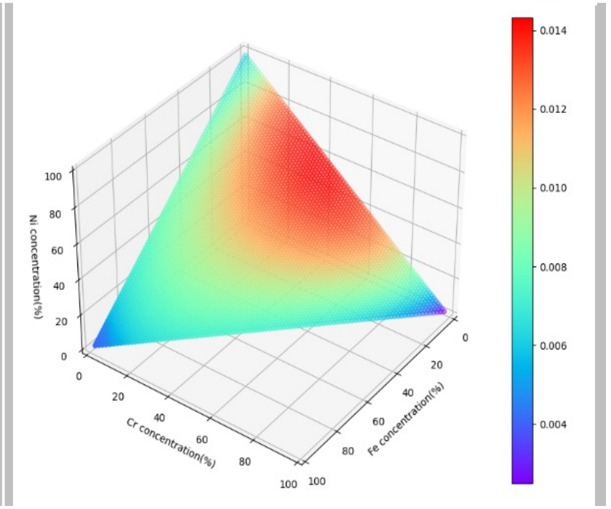
**Cr, Fe ≤ 20**
**Ni ≥ 80**



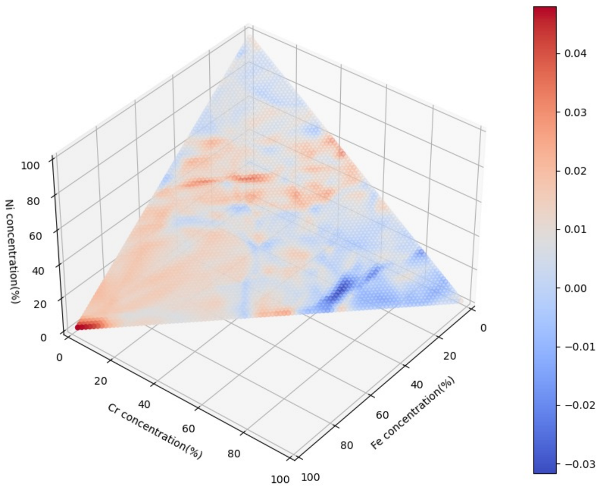
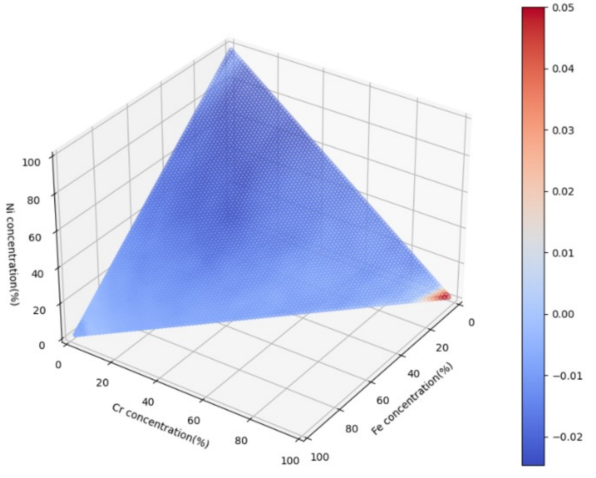
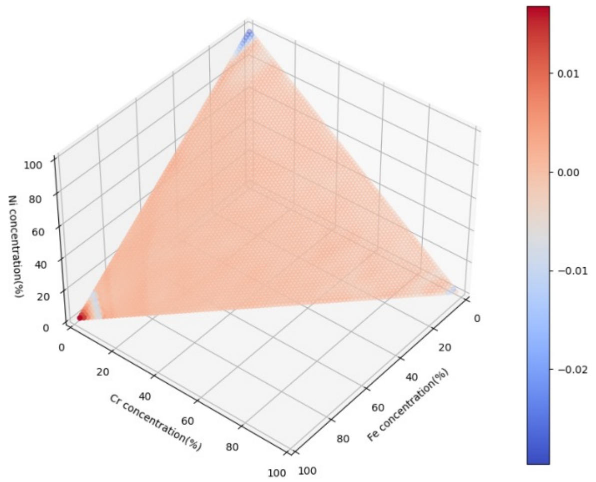

Train : 700
Test : 259
Validation : 41

959

# Result and discussion

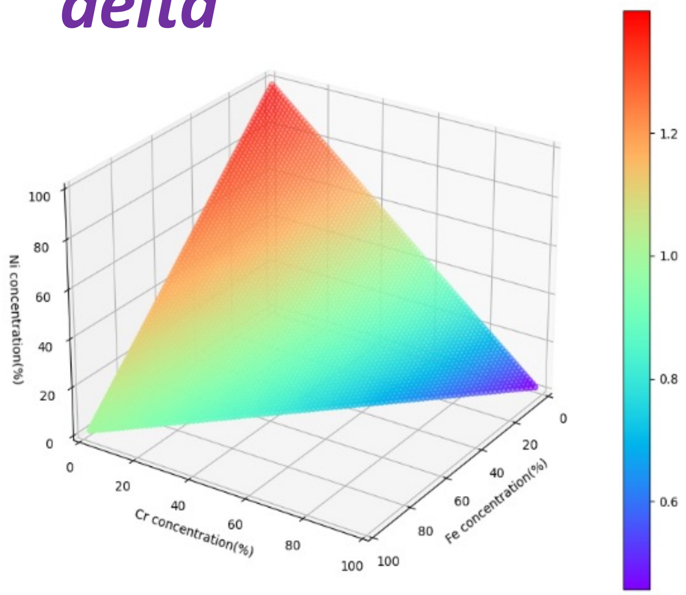
| | Model 1 | Model 2 | Model 3 |
|---|---|---|---|
| delta |  |  |  |
| Average Atomic Shear Strain |  |  |  |

# Result and discussion

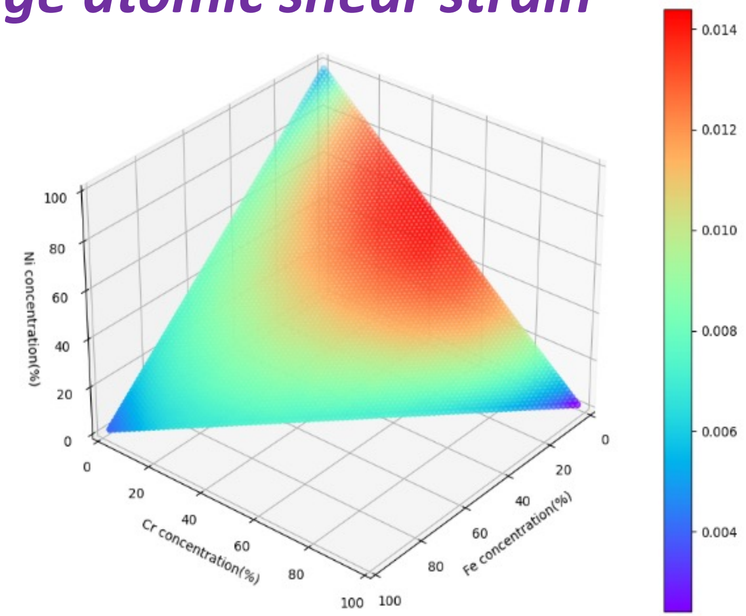
| | Model 1 | Model 2 | Model 3 |
|---|---|---|---|
| Delta error |  |  |  |

# Result and discussion

## *delta*




## *Average atomic shear strain*





① Zhang, Y., Zhou, Y. J., Lin, J. P., Chen, G. L., & Liaw, P. K. (2008). *Solid-Solution Phase Formation Rules for Multi-component Alloys. Advanced Engineering Materials, 10(6), 534–538.* doi:10.1002/adem.200700240 原子半徑

② GUO, S., & LIU, C. T. (2011). *Phase stability in high entropy alloys: Formation of solid-solution phase or amorphous phase. Progress in Natural Science: Materials International, 21(6), 433–446.* doi:10.1016/s1002-0071(12)60080-x 原子半徑、電子性質

③ Dai, F.-Z., Sun, Y., Wen, B., Xiang, H., & Zhou, Y. (2020). Temperature Dependent Thermal and Elastic Properties of High Entropy (Ti0.2Zr0.2Hf0.2Nb0.2Ta0.2)B2: Molecular Dynamics Simulation by Deep Learning Potential. Journal of Materials Science & Technology. **用AASS去衡量高熵二硼化物的lattice distortion**

# Result and discussion

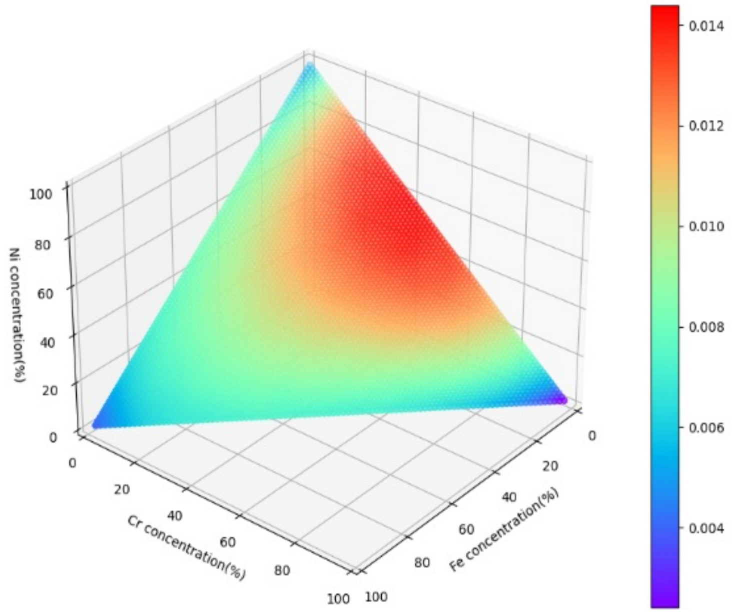
**Application on dislocation energy barrier calculation …**

Composition

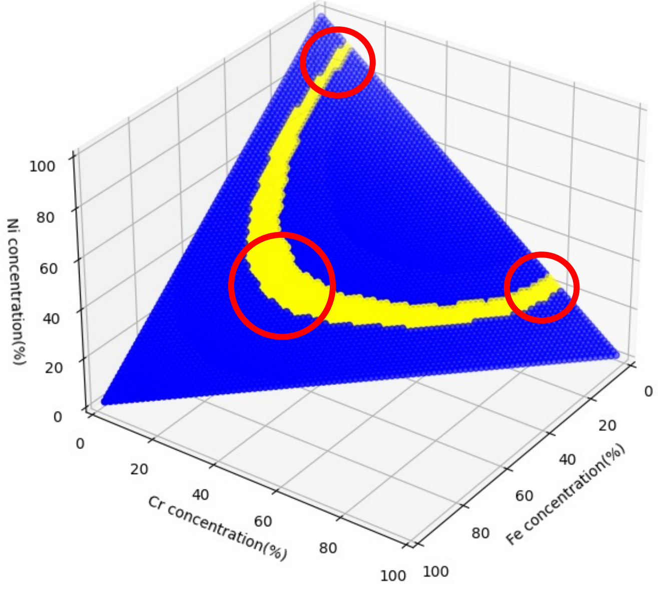
Distortion

Internal stress

Energy barrier




AASS at 0.0095 ~ 0.0105



# End