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Computational Modeling and Structure Visualization of Ni_2X_3 (X= Cr, Ti, W, Co and C) Structure Type Possibility of Cast Ni-Base Superalloy

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ABSTRACT

New trend of structural modeling and visualization investigations were performed on Ni base super-alloy to show the possibility of forming Ni_2X_3 structure type with P_{41212} space group as minor phase inside nickel matrix .Ni base super-alloy specimen could be structurally formed as M_2X_3 structure type where M-sites occupy by Nickel-atoms and X-sites occupy by (X = Cr, Ti, W, Co and C) with total molar ratios = 3 mole. The Ni-specimens were cast under different superheat levels and various cooling rates. Structural investigations specially bond distances measurements and torsion on angles indicated that nickel has four different types nominated as Ni_1,Ni_2 , Ni_3 and Ni_4 while chromium has three different types inside the unit cell of Ni_2X_3 . The validity of structure was investigated carefully by construction 3x3x3 super-unit cell and studying the torsion on angles on its stability.

Keywords: Computational Modeling; Visualization; XRD-Profile; Bond distances.

INTRODUCTION

The Ni -base alloy has a great attention of researchers and investigators due to their industrial and manufacturing application as blades of powerful gas turbines (over 125MW). These blades work at critical conditions of creep, corrosion, and fatigue for more than 70,000h. Many of additives specially refractory elements like Mo, W, Ta, Cr and Co were added to prevent local hot corrosion [1-3]. In spite of important role of most of Ni base super-alloy in the high temperature performance, limited data on microstructure and material characterization are reported, therefore a complete description of the effect of casting parameters on the Ni base

alloys is required [4,5-7]. Ni base super-alloy is known to have a multiphase microstructure consisting of a solid solution strengthened austenitic nickel γ matrix, bimodal γ' precipitate, γ / γ' eutectic, carbides and a small amount of deleterious phases such as: δ , σ , η and laves [8-11]. In some cases, minor phases like η phase and σ phase which usually form at solid state in superalloys may form at the end of solidification owing to the influence of composition. The η phase has a hexagonal close-packed (hcp) structure and has the basic stoichiometry of Ni₃Ti, while σ phase has a tetragonal topologically close-packed (TCP) structure. Bouse has reported that η phase or platelet phases formed in the as cast microstructure of alloys containing high percentages of Ti, such as IN792_Hf, IN939, GTD111 and IN6203 [12]. Other studies also reported the occurrence of η phase at the periphery of the γ / γ' eutectics [13-15].

Many researchers investigated the suggestion of existing species like oxides, hydroxides, oxy hydroxides, nitrates, nitrides, sulfates, chlorides and oxy chlorides of Fe ,Cr and Ni could be present in the passive film and surface layers of synthesized M-based-alloy [16-25] . The contributions of other elements apart from Ti ,W, Al, Mo and Co, were not expected to be detected in surface layer, since their content in the alloy was very low to be detectable although it form some crystalline phases with the nickel which is the major component of the alloy.

The major goal of the present article is visualization on the basis of molecular structure of Ni_2X_3 structure to prove the possibility of this structure type to be present together in the nickelmatrix of cast Ni-superalloy.

MATERIALS AND METHODS

II.I. Experimental :

The Ni-based alloy used in this work was received as turbine blade scrap supplied from a gas turbine power plant. Table 1 shows the chemical composition of as-received alloy. This scrap was double melted and cast under vacuum using an induction vacuum furnace. In the second melt some amounts of alloying elements such as Ti, Co, Cr, W and C were added to adopt the chemical composition, then a third melting was made to ensure melting and homogenous distribution of all alloying elements in the heat. Heats were made by melting 10 kg of turbine blade scrap. Pouring was carried out into an investment casting ceramic mold.

The chemical composition as well as XRD of the prepared experimental polycrystalline Ni base super-alloy is shown in Table 1 as atomic weight percentage and Fig.1 for samples with two different heat treatment cycles .

II.II. Computational Investigations :

A visualized studies of crystal structure were made by using Diamond Molecular Structure version 3.2 package, Germany and Mercury 2.3-BUILD RC4-UK .

A visualization study made is concerned by matching and comparison of experimental and theoretical data of atomic positions ,bond distances , oxidation states and bond torsion on the crystal structure formed . Some of these data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif, or by emailing data_request @ccdc.cam.ac.uk, or by contacting ICSD-Fiz-Karlsruhe-Germany.

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RESULTS AND DISCUSSION

III.I-Structure Identification :

Generally it is well known that x-ray diffraction measurements for nickel alloy is not valid as absolute analytical tool but it applied as complementary tools to confirm the internal structure of investigated alloy whatever the metallic alloy composition is . As clear in Fig.1 the most intense reflection peak (I_0) for Ni-superalloy lies at two theta ~ 41° in both diffractograms recorded although the differences in heat treatment cycles .This is a good evidence that heat treatments or cooling rates has limited impact on the major phase of Ni-superalloy as shown in Fig.1.



Fig.1 Experimental XRD-profile recorded for Ni-superalloy with two different heat treatments

Red diffractogram is differ than blue diffractogram in thermal treatment and cooling rates although from these differences the assigned peaks for each patterns are nearly identical which confirms casting conditions have a limited impact on the main crystal form but not to the minor phases as Ni_2X_3 which is the main phase structure in these investigations .Micro-structural features of Ni-super alloy as a function in heat treatments and cooling rates will be investigated deeply in the near advance in another manuscript.

The selected ranges of two theta must be within $40-45^{\circ}$ in which maximum intense reflection peak I_{o} is lying in .

III.II. Structure Analyses and Visualization Structural Features of Ni₂X₃ :

Fig.2 represents the visualized tetragonal unit cell of Ni-superalloy with simulated crystal structure Ni_2X_3 where x = Cr, C, Ti, Co and W. The unit cell diagramed with 80 atoms , eight symmetry operations ,64 cell corners ,144 edges and eleven atomic parameters .

The analysis of structure features inside the visualized unit cell are concerned by bond distances , angles, angles torsion and symmetry operation .It was found that there are three types of chromium atoms symbolized as Cr1, Cr2 and Cr3, four types for nickel



Tetragonal Unit Cell of Ni2X3-alloy with P41212 Space Group

Fig.2 : Tetragonal unit cell of visualized Ni₂X₃ structure .

atoms symbolized as Ni₁ ,Ni₂,Ni₃ and Ni₄ . Furthermore it was observed only one type for titanium, carbon, tungsten and cobalt .The analyses of Tables (3-9) will enhance us to understand that the possibility of forming Ni₂X₃ crystal structure with P_{42121} space group where x = Cr ,C ,Ti, Co and W is valid inside Ni-alloy matrix even it formed as minor phase . Table.3 reported some selected bond distances and angle concerning by chromium type one (Cr1). As it clear seven bond distances are recorded according to the following sequence Cr1-Ni2 ,Cr1-Ni1 ,Cr1-Co1,Cr1-Ti1,Cr1-Ti1,Cr1-W1,Cr1-Cr2 and finally Cr1-Cr3 with bond distances equal to 2.7302 ,3.0240 ,3.6210 ,3.3963 ,3.6297 ,3.5263 and finally 3.3965 Å respectively .From these bond distances for chromium atoms are different Cr1-Cr2 =3.5263 while Cr1-Cr3=3.3965 Å .Another good notification is the minimum bond length is for Cr1-Ni2= 2.7302 Å and maximum one for Cr1-Ti1 = 3.6297 Å that could be due to that Ni2 is lower oxidation state for nickel = +I while Cr1 is in higher oxidation state for chrome = +VI.

Table.4 is displaying the bond distances recorded for chromium type two (Cr2) with the surrounding neighboring atoms starting with nickel atoms Ni1,Ni2 since Cr2-Ni1= 2.8117 while Cr2-Ni2 = 2.8523 Å the difference in bond length confirm that nickel has two different oxidation state speculate to be +I and +II .The rest regular data were recorded for Cr2 with Co1,C1 and Ti1 with bond lengths equal to 3.8026, 3.6727 and finally Cr2-Ti1 = 3.4500 Å . It was noticeable also that Cr2 linked with other two types of chrome Cr1 and Cr3 recording 3.5263 Å for Cr2-Cr1 and 3.8199 Å is for Cr2-Cr3 which confirm that chrome has more than oxidation state inside unit cell of crystal structure .From Table.5 one can deduces many observations titanium (Ti1) is bonded to four different types of nickel namely Ni1,Ni2,Ni3 and Ni4 with values 2.7258, 3.147, 2.9202 and 3.0876 Å respectively .

These values of bond distances recorded are a good evidence for existence four different averaged oxidation state on nickel atoms .The same were noticeable with different chromium

atoms Cr1,Cr2 and Cr3 which confirm chrome has three or more different oxidation state as mentioned before .

The tungsten bonding was described as shown in Table.6 , it was observed that tungsten was bonded to all atoms types inside the crystal lattice without violation only chrome type two bond (Cr2-W) was absent .Tungsten symbolized as (W1) was bonded to the four types of nickel recoding minimum with Ni1 (W1-Ni1 = 2.9146 Å) and maximum with Ni4 (W1-Ni4 = 3.037 Å) .The most interested phenomenon appears in tungsten bonding inside the crystal lattice is appearing two different values for each bonding with Co1,C1and Ti1 respectively . This notification could interpretable if the average oxidation state varies according to the neighboring atoms environment which is actually occurred in the present investigations .

Table.8 describes the bond distances recorded for carbon atoms (C1) .From tabulated bond length it is clear that carbon is bonded to all kind of atoms in the crystal lattice without violation only C1-Cr1 is absent since it bonded to the four different types of nickel with minimum bond length 2.8174 Å (C1-Ni3) and maximum bond length recorded for (C1-Ni1,Ni4) with bond length = 2.9714 Å . Carbon is bonded to two types of chrome (Cr2,Cr3) with bond length nearly equal~ 2.6727 Å .

The analysis of Table.9 indicated that nickel atoms type one (Ni1) is linked systematically to the three types of chromium Cr1,Cr2 and Cr3 with bond distances 3.0242 ,2.8117 and 2.865 Å respectively .One can observe that the difference between Ni1-Cr2 and Ni1-Cr3 is very closed nearly ~ 0.05 Å which confirm that Cr2 and Cr3 nearly have the same oxidation state in some points inside the crystalline structure . The second notification is absence of Ni1-Ni3 boding while Ni1-Ni2 and Ni1-Ni4 are present with bond distances equal to 2,5127 and 2.5607 Å respectively .The third observation is linking to the whole rest atom in the Ni₂X₃ lattice such as Co1,C1,W1 and Ti1 with bonds equal to 2.6580 ,2.9714 ,2.9114 and finally Ni1-Ti1 with 2.7258 Å respectively .



(b) Zoom in focused view for two theta range $(40 - 45^\circ)$.

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Fig._{3a} displays the visualized XRD-profile of Ni₂X₃ structure with P₄₁₂₁₂ space group. It was notified that the numbers of peaks per pattern was ~ more than 100 lines due to polycrystalline phases induce together into the nickel alloy matrix with evaluated Ni₂X₃ phase . To clarify whether or not maximum intense peak (I_o) which lies at 2 theta ~41°) of Ni₂X₃ phase is present or not Fig._{3b} was constructed to increase the resolution of overlapped peaks . From Fig.3b it was obviously that maximum intense peak (I_o) which lies at 2 theta ~ 41° is actually present with good fitting with experimental one .



3x3x3 Super Unit Cell of Tetragonal Ni2X3 Structure Type with P41212 Space Group

Fig.4: 3x3x3 super unit cell of Ni₂X₃ type structure

Table 1. Chemical composition of as cast Ni base super-alloys

| Elements Alloy | С | Cr | W | Ti | Со | Ni |
|-------------------|------|-------|------|------|-------|------|
| Ni-Based-Alloy | 0.13 | 15.01 | 2.81 | 3.63 | 7.67 | Bal. |
| As cast (H) | 0.54 | 16.95 | 4.36 | 5.88 | 10.48 | Bal. |

III.III. Structure Validity of Ni₂X₃ :

The matching between experimental and visualized XRD-profile of Ni₂X₃ type structure enhances the validity and stability of this structure to be real as proved in present investigations. To confirm this trend 3x3x3 super lattice was constructed to measure the torsion on bonds and angles as clear in Fig.4 and it was observed that there is no violation on torsion angles inside the crystal lattice accompanied with increasing in stability constant of this structure \cdot . To confirm the validity of this structure type Ni₂X₃ the torsion angles inside the super unit cell were analyzed carefully, the maximum and minimum angles were reported and compared as follow table.3 the max. angle found was 139° for Ni4-Ni1-Ti1 while minimum one 56.2° is for Ni4-Ni4-Co1 .From table.4 only high torsion was observed on angle Cr2-Ni1-Co1 which equal 44.31° .Table five has recorded maximum angle 173.86° with symmetry operation (x, y, z) and minimum angle (maximum torsion) is recorded for Ti1-Ni1-Co1 ~ 44.25° with symmetry operation (x, 1+y, z).

| No. | 2 | dÅ | Intensity | h | k | l | Mult. |
|-----|--------|--------|-------------|---|---|----|-------|
| 61 | 40.106 | 2.2465 | 14258465.57 | 1 | 3 | 0 | 8 |
| 62 | 40.185 | 2.2423 | 4474278.10 | 1 | 3 | 1 | 16 |
| 63 | 40.421 | 2.2297 | 18211404.40 | 1 | 3 | 2 | 16 |
| 64 | 40.811 | 2.2093 | 25404942.81 | 1 | 3 | 3 | 16 |
| 65 | 40.847 | 2.2074 | 689608.52 | 0 | 3 | 6 | 8 |
| 66 | 40.875 | 2.2060 | 4560857.81 | 0 | 2 | 13 | 8 |
| 67 | 40.961 | 2.2015 | 101425.55 | 2 | 2 | 8 | 8 |
| 68 | 40.993 | 2.1999 | 1319116.41 | 1 | 2 | 12 | 16 |
| 69 | 41.103 | 2.1943 | 2102784.77 | 1 | 1 | 15 | 8 |
| 70 | 41.352 | 2.1817 | 7024742.85 | 1 | 3 | 4 | 16 |
| 71 | 41.447 | 2.1769 | 719.76 | 0 | 1 | 16 | 8 |
| 72 | 41.847 | 2.1570 | 1032578.09 | 0 | 3 | 7 | 8 |
| 73 | 42.039 | 2.1476 | 5718493.88 | 1 | 3 | 5 | 16 |
| 74 | 42.262 | 2.1368 | 272326.69 | 2 | 2 | 9 | 8 |
| 75 | 42.867 | 2.1080 | 680774.65 | 1 | 3 | 6 | 16 |
| 76 | 42.893 | 2.1068 | 16865192.06 | 1 | 2 | 13 | 16 |
| 77 | 42.928 | 2.1051 | 499060.64 | 0 | 2 | 14 | 8 |
| 78 | 42.976 | 2.1029 | 2314106.00 | 0 | 3 | 8 | 8 |
| 79 | 43.443 | 2.0813 | 110913.53 | 1 | 1 | 16 | 8 |
| 80 | 43.677 | 2.0707 | 765484.18 | 2 | 2 | 10 | 8 |

 $Table.2: Selected \ data \ of \ visualized \ XRD-diffraction \ for \ Ni_2X_3 \ structure$

Table.3 : Selected structural parameters for Ni-type 4 atoms inside unit cell of Ni_2X_3 .

| Atom1 | Atom2 | Sym.Op.1 | d1-2Å | Atom3 | Sym.Op.2 | d1-3Å | Angle213 |
|-------|-------|-----------|--------|-------|-----------------------|--------|----------|
| Ni4 | Ni1 | x, 1+y, z | 2.5607 | Ni3 | 1.5-x, 0.5+y, 0.25-z | 2.7506 | 115.157 |
| | Ni1 | x, 1+y, z | 2.5607 | C1 | 0.5-x, 0.5+y, 0.25-z | 2.9599 | 122.252 |
| | Ni1 | x, 1+y, z | 2.5607 | C1 | x, 1+y, z | 2.9770 | 64.388 |
| | Ni1 | x, 1+y, z | 2.5607 | Co1 | 0.5-x, 0.5+y, 0.25-z | 3.0166 | 140.235 |
| | Ni1 | x, 1+y, z | 2.5607 | Co1 | x, 1+y, z | 3.0167 | 56.209 |
| | Ni1 | x, 1+y, z | 2.5607 | W1 | x, y, z | 3.0397 | 62.028 |
| | Ni1 | x, 1+y, z | 2.5607 | Ti1 | x, y, z | 3.0876 | 56.793 |
| | Ni1 | x, 1+y, z | 2.5607 | Ti1 | 0.5-x, 0.5+y, 0.25-z | 3.1030 | 139.024 |
| | Ni1 | x, 1+y, z | 2.5607 | Ni4 | 0.5-x, -0.5+y, 0.25-z | 3.7383 | 109.352 |
| | Ni1 | x, 1+y, z | 2.5607 | Ni4 | 0.5-x, 0.5+y, 0.25-z | 3.7383 | 88.445 |

Table.4 : Selected bond distances for Cr-type 2 atoms inside unit cell of Ni_2X_3 .

| Atom1 | Atom2 | Sym.Op.1 | d1-2Å | Atom3 | Sym.Op.2 | d1-3Å | Angle213 |
|-------|-------|----------|--------|-------|---------------|--------|----------|
| Cr2 | Ni1 | y, x, -z | 2.8117 | Ni1 | x, y, z | 2.8117 | 111.258 |
| | Ni1 | y, x, -z | 2.8117 | Ni2 | x, y, z | 2.8523 | 143.076 |
| | Ni1 | у, х, -z | 2.8117 | Ni2 | у, х, -z | 2.8523 | 52.660 |
| | Ni1 | у, х, -z | 2.8117 | Ti1 | x, y, z | 3.4525 | 99.338 |
| | Ni1 | y, x, -z | 2.8117 | Ti1 | у, х, -z | 3.4525 | 98.429 |
| | Ni1 | y, x, -z | 2.8117 | Cr1 | -1+x, -1+y, z | 3.5263 | 55.629 |
| | Ni1 | у, х, -z | 2.8117 | Cr3 | x, y, z | 3.5883 | 147.832 |
| | Ni1 | у, х, -z | 2.8117 | Cr3 | y, x, -z | 3.5883 | 96.668 |
| | Ni1 | у, х, -z | 2.8117 | C1 | y, x, -z | 3.6727 | 52.526 |
| | Ni1 | у, х, -z | 2.8117 | C1 | x, y, z | 3.6727 | 150.388 |
| | Ni1 | y, x, -z | 2.8117 | Co1 | x, y, z | 3.8026 | 91.771 |
| | Ni1 | у, х, -z | 2.8117 | Co1 | у, х, -z | 3.8026 | 44.314 |
| | Ni1 | у, х, -z | 2.8117 | Cr3 | -1+x, y, z | 3.8199 | 48.948 |

| Ni1 | у, х, -z | 2.8117 | Cr3 | y, -1+x, -z | 3.8199 | 94.369 |
|-----|----------|--------|-----|---------------|--------|---------|
| Ni1 | x, y, z | 2.8117 | Ni2 | x, y, z | 2.8523 | 52.660 |
| Ni1 | x, y, z | 2.8117 | Ni2 | у, х, -z | 2.8523 | 143.076 |
| Ni1 | x, y, z | 2.8117 | Ti1 | x, y, z | 3.4525 | 98.429 |
| Ni1 | x, y, z | 2.8117 | Ti1 | y, x, -z | 3.4525 | 99.338 |
| Ni1 | x, y, z | 2.8117 | Cr1 | -1+x, -1+y, z | 3.5263 | 55.629 |
| Ni1 | x, y, z | 2.8117 | Cr3 | x, y, z | 3.5883 | 96.668 |
| Ni1 | x, y, z | 2.8117 | Cr3 | у, х, -z | 3.5883 | 147.832 |
| Ni1 | x, y, z | 2.8117 | C1 | у, х, -z | 3.6727 | 150.388 |
| Ni1 | x, y, z | 2.8117 | C1 | x, y, z | 3.6727 | 52.526 |

Table.5: Selected structural parameters for Ti-type 1 atoms inside unit cell of Ni_2X_3 .

| Atom1 | Atom2 | Sym.Op.1 | d1-2Å | Atom3 | Sym.Op.2 | d1-3Å | Angle213 |
|-------|-------|------------|--------|-------|------------|--------|----------|
| Ti1 | Ni1 | x, 1+y, z | 2.7258 | Ni3 | -1+x, y, z | 2.9202 | 135.353 |
| | Ni1 | x, 1+y, z | 2.7258 | Ni4 | x, y, z | 3.0876 | 51.814 |
| | Ni1 | x, 1+y, z | 2.7258 | Ni2 | у, х, -z | 3.1479 | 87.362 |
| | Ni1 | x, 1+y, z | 2.7258 | Cr1 | -1+x, y, z | 3.3963 | 57.972 |
| | Ni1 | x, 1+y, z | 2.7258 | Cr3 | -1+x, y, z | 3.4228 | 128.236 |
| | Ni1 | x, 1+y, z | 2.7258 | Cr2 | x, y, z | 3.4525 | 114.598 |
| | Ni1 | x, 1+y, z | 2.7258 | Cr3 | у, х, -z | 3.5342 | 53.239 |
| | Ni1 | x, 1+y, z | 2.7258 | W1 | x, y, z | 3.5863 | 52.888 |
| | Ni1 | x, 1+y, z | 2.7258 | Co1 | x, y, z | 3.7552 | 173.862 |
| | Ni1 | x, 1+y, z | 2.7258 | C1 | x, y, z | 3.7809 | 115.287 |
| | Ni1 | x, 1+y, z | 2.7258 | Co1 | x, 1+y, z | 3.8086 | 44.258 |
| | Ni1 | x, 1+y, z | 2.7258 | W1 | -1+x, y, z | 3.8313 | 98.369 |
| | Ni3 | -1+x, y, z | 2.9202 | Ni4 | x, y, z | 3.0876 | 100.453 |
| | Ni3 | -1+x, y, z | 2.9202 | Ni2 | у, х, -z | 3.1479 | 111.193 |
| | Ni3 | -1+x, y, z | 2.9202 | Cr1 | -1+x, y, z | 3.3963 | 103.471 |
| | Ni3 | -1+x, y, z | 2.9202 | Cr3 | -1+x, y, z | 3.4228 | 59.110 |
| | Ni3 | -1+x, y, z | 2.9202 | Cr2 | x, y, z | 3.4525 | 108.217 |
| | Ni3 | -1+x, y, z | 2.9202 | Cr3 | у, х, -z | 3.5342 | 159.089 |
| | Ni3 | -1+x, y, z | 2.9202 | W1 | x, y, z | 3.5863 | 143.161 |
| | Ni3 | -1+x, y, z | 2.9202 | Co1 | x, y, z | 3.7552 | 48.529 |
| | Ni3 | -1+x, y, z | 2.9202 | C1 | x, y, z | 3.7809 | 95.911 |

Table.6: Selected bond distances for W-type 1 atoms inside unit cell of Ni_2X_3 .

| Atom1 | Atom2 | Sym.Op.1 | d1-2Å | Atom3 | Sym.Op.2 | d1-3Å | Angle213 |
|-------|-------|-----------|--------|-------|-------------|--------|----------|
| W1 | Ni2 | x, 1+y, z | 2.7009 | Ni3 | x, y, z | 2.7144 | 150.174 |
| | Ni2 | x, 1+y, z | 2.7009 | Ni1 | x, 1+y, z | 2.9146 | 52.990 |
| | Ni2 | x, 1+y, z | 2.7009 | Ni4 | x, y, z | 3.0397 | 93.078 |
| | Ni2 | x, 1+y, z | 2.7009 | Cr3 | y, x, -z | 3.4252 | 55.244 |
| | Ni2 | x, 1+y, z | 2.7009 | Ti1 | x, y, z | 3.5863 | 96.965 |
| | Ni2 | x, 1+y, z | 2.7009 | Cr1 | x, y, z | 3.6264 | 48.455 |
| | Ni2 | x, 1+y, z | 2.7009 | Co1 | 1+x, 1+y, z | 3.6853 | 62.254 |
| | Ni2 | x, 1+y, z | 2.7009 | C1 | x, 1+y, z | 3.7275 | 51.947 |
| | Ni2 | x, 1+y, z | 2.7009 | C1 | x, y, z | 3.8211 | 150.531 |
| | Ni2 | x, 1+y, z | 2.7009 | Ti1 | 1+x, y, z | 3.8313 | 100.758 |
| | Ni3 | x, y, z | 2.7144 | Ni1 | x, 1+y, z | 2.9146 | 155.946 |
| | Ni3 | x, y, z | 2.7144 | Ni4 | x, y, z | 3.0397 | 114.119 |
| | Ni3 | x, y, z | 2.7144 | Cr3 | x, y, z | 3.4197 | 60.711 |
| | Ni3 | x, y, z | 2.7144 | Cr3 | y, x, -z | 3.4252 | 125.521 |
| | Ni3 | x, y, z | 2.7144 | Ti1 | x, y, z | 3.5863 | 108.453 |

| Ni3 | x, y, z | 2.7144 | Cr1 | x, y, z | 3.6264 | 102.211 |
|-----|---------|--------|-----|-------------|--------|---------|
| Ni3 | x, y, z | 2.7144 | Co1 | 1+x, 1+y, z | 3.6853 | 97.463 |
| Ni3 | x, y, z | 2.7144 | C1 | x, 1+y, z | 3.7275 | 138.861 |
| Ni3 | x, y, z | 2.7144 | C1 | x, y, z | 3.8211 | 47.439 |
| Ni3 | x, y, z | 2.7144 | Ti1 | 1+x, y, z | 3.8313 | 49.460 |

Table.7: Selected structural parameters for Co-type 1 atoms inside unit cell of Ni_2X_3 .

| Atom1 | Atom2 | Sym.Op.1 | d1-2Å | Atom3 | Sym.Op.2 | d1-3Å | Angle213 |
|-------|-------|----------|--------|-------|---------------|--------|----------|
| Co1 | Ni1 | x, y, z | 2.6580 | Ni3 | -1+x, y, z | 2.8470 | 144.465 |
| | Ni1 | x, y, z | 2.6580 | Ni4 | x, -1+y, z | 3.0167 | 53.192 |
| | Ni1 | x, y, z | 2.6580 | Cr1 | -1+x, -1+y, z | 3.2610 | 60.436 |
| | Ni1 | x, y, z | 2.6580 | Ni2 | -1+x, y, z | 3.4071 | 108.701 |
| | Ni1 | x, y, z | 2.6580 | Cr3 | -1+x, y, z | 3.4469 | 106.445 |
| | Ni1 | x, y, z | 2.6580 | W1 | -1+x, -1+y, z | 3.6853 | 103.288 |
| | Ni1 | x, y, z | 2.6580 | C1 | x, y, z | 3.6872 | 52.872 |
| | Ni1 | x, y, z | 2.6580 | C1 | -1+x, y, z | 3.7144 | 157.530 |
| | Ni1 | x, y, z | 2.6580 | Ti1 | x, y, z | 3.7552 | 94.321 |
| | Ni1 | x, y, z | 2.6580 | Cr2 | x, y, z | 3.8026 | 47.645 |
| | Ni1 | x, y, z | 2.6580 | Ti1 | x, -1+y, z | 3.8086 | 45.701 |

Table.8 Selected bond distances for C -type 1 atoms inside unit cell of Ni_2X_3 .

| Atom1 | Atom2 | Sym.Op.1 | d1-2Å | Atom3 | Sym.Op.2 | d1-3Å | Angle213 |
|-------|-------|----------|--------|-------|-----------------------|--------|----------|
| C1 | Ni3 | x, y, z | 2.8174 | Ni4 | 0.5-x, -0.5+y, 0.25-z | 2.9599 | 114.879 |
| | Ni3 | x, y, z | 2.8174 | Ni2 | x, y, z | 2.9627 | 95.096 |
| | Ni3 | x, y, z | 2.8174 | Ni1 | x, y, z | 2.9714 | 145.192 |
| | Ni3 | x, y, z | 2.8174 | Ni4 | x, -1+y, z | 2.9770 | 144.261 |
| | Ni3 | x, y, z | 2.8174 | Ni3 | 1.5-x, -0.5+y, 0.25-z | 3.0866 | 90.441 |
| | Ni3 | x, y, z | 2.8174 | Cr2 | x, y, z | 3.6727 | 111.682 |
| | Ni3 | x, y, z | 2.8174 | Cr3 | x, y, z | 3.6777 | 56.351 |
| | Ni3 | x, y, z | 2.8174 | Co1 | x, y, z | 3.6872 | 161.28 |
| | Ni3 | x, y, z | 2.8174 | Co1 | 1+x, y, z | 3.7144 | 49.368 |
| | Ni3 | x, y, z | 2.8174 | W1 | x, -1+y, z | 3.7275 | 108.69 |
| | Ni3 | x, y, z | 2.8174 | Ti1 | x, y, z | 3.7809 | 101.26 |
| | Ni3 | x, y, z | 2.8174 | W1 | x, y, z | 3.8211 | 45.205 |
| | Ni3 | x, y, z | 2.8174 | Co1 | 0.5-x, 0.5+y, 0.25-z | 3.8563 | 66.069 |
| | Ni3 | x, y, z | 2.8174 | Ti1 | 0.5-x, -0.5+y, 0.25-z | 3.8747 | 108.365 |

From Tables 6, 7,8 and 9 it was observed that the maximum torsion angles were found to be 47.43, 45.7, 45.2 and 47.68° for W1-Ni3-C1 ,Co1-Ni1-Ti1 ,C1-Ni3-W1 and Cr1-Ni2-Cr3 respectively. Theses torsion angles are actually not affected too much on the main crystal structure of the domain metallic alloy due to Ni-super alloy is mainly metallic alloy and the crystalline phases present in the Ni-matrix are minor phases found together on the major nickel matrix .

Table.9: Selected structural parameters for Cr-type 1 atoms inside unit cell of $\mathrm{Ni}_2 X_3$.

| Atom1 | Atom2 | Sym.Op.1 | d ₁₋₂ Å | Atom3 | Sym.Op.2 | d ₁₋₃ Å | Angle213 |
|-------|-------|-----------|--------------------|-------|--------------|--------------------|----------|
| Cr1 | Ni2 | x, 1+y, z | 2.7302 | Ni2 | 1+y, x, -z | 2.7302 | 136.591 |
| | Ni2 | x, 1+y, z | 2.7302 | Ni1 | 1+x, 1+y, z | 3.0242 | 118.505 |
| | Ni2 | x, 1+y, z | 2.7302 | Ni1 | 1+y, 1+x, -z | 3.0242 | 89.827 |
| | Ni2 | x, 1+y, z | 2.7302 | Co1 | 1+y, 1+x, -z | 3.2610 | 129.849 |
| | Ni2 | x, 1+y, z | 2.7302 | Co1 | 1+x, 1+y, z | 3.2610 | 68.660 |

| Ni2 | x, 1+y, z | 2.7302 | Ti1 | y, 1+x, -z | 3.3963 | 60.687 |
|-----|-----------|--------|-----|-------------|--------|---------|
| Ni2 | x, 1+y, z | 2.7302 | Ti1 | 1+x, y, z | 3.3963 | 111.669 |
| Ni2 | x, 1+y, z | 2.7302 | Cr2 | 1+x, 1+y, z | 3.5263 | 111.704 |
| Ni2 | x, 1+y, z | 2.7302 | W1 | y, x, -z | 3.6264 | 99.975 |
| Ni2 | x, 1+y, z | 2.7302 | Cr3 | x, 1+y, z | 3.6297 | 48.498 |
| Ni2 | x, 1+y, z | 2.7302 | Cr3 | 1+y, x, -z | 3.6297 | 168.812 |
| Ni2 | x, 1+y, z | 2.7302 | Cr3 | x, y, z | 3.9365 | 91.313 |
| Ni2 | x, 1+y, z | 2.7302 | Cr3 | y, x, -z | 3.9365 | 47.684 |

CONCLUSION

The conclusive remarks inside present manuscript can summarized as follow ;

- 1- The visualization confirmed the possibility of modeled Ni₂X₃ structure type with P_{41212} space group as minor phase on Ni base super-alloy.
- 2- Studies proved that Ni base super-alloy specimen could be structurally formed as M_2X_3 structure type where M-sites occupy by Nickel-atoms and X-sites occupy by (X= Cr, Ti, W, Co and C) with total molar ratios = 3 mole .
- 3- Structural investigations specially bond distances measurements confirmed that nickel has four different types nominated as Ni_1, Ni_2, Ni_3 and Ni_4 while chromium has three different types inside the unit cell of Ni_2X_3 .
- 4- The validity of modeled Ni_2X_3 structure type with P_{41212} space group was confirmed through torsion calculations on the main angles carefully of $3x_3x_3$ super-unit cell.

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