Data Article

Data sets of predicted stable and meta-stable crystalline phase structural of NB-N system under pressure

Diego Restrepo-Leal, José Sierra-Ortega*, Gene Elizabeth Escorcia-Salas

Grupo de Investigación en Teoría de la Materia Condensada, Universidad del Magdalena, Facultad de Ciencias Básicas, Carrera 32 No 22 – 08, Santa Marta, Colombia

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ABSTRACT

This document presents a dataset on various stoichiometric Niobium nitrides compounds under different pressures, which have been identified by first-principles calculations in combination with an evolutionary algorithm methodology implemented in the USPEX code in its variable-composition mode. The feature of this methodology is to find the ground state or metastable structures with only the knowledge of chemical composition at given pressure conditions and predict through all possible structures, not relying on any prior known structural information. We have successfully predicted the crystal structures and phase transitions of NbN at pressures up to 100 GPa. Because the Niobium nitrides represent a rich family of phases where the stability and microstructures are still not completely understood, it is exciting to find news structures of NbₓNᵧ under high pressure.

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* Corresponding author.
E-mail addresses: diegorestrepoal@unimagdalena.edu.co (D. Restrepo-Leal), jcsierra@unimagdalena.edu.co (J. Sierra-Ortega), gescorcia@unimagdalena.edu.co (G.E. Escorcia-Salas).

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Specifications Table

| Subject | Materials Science. |
|---|---|
| Specific subject area | Materials Science (General), Metals and Alloys, Computer Science Applications. |
| Type of data | Table, Figures. |
| How data were acquired | The stable crystal structures and compositions of Nb$_x$N$_y$ compounds at 0, 30, 50, and 100 GPa were predicted by using the evolutionary algorithm USPEX (Universal Structure Predictor: Evolutionary Xtallography) software together with the Quantum-ESPRESSO package. Stable compositions were determined using the convex hull construction; taking into account that a compound is thermodynamically stable when its enthalpy of formation from the elements and from any other compounds is negative. Formation enthalpy calculations and structure relaxations were performed by using density functional theory (DFT) within the Perdew-Burke-Ernzerhof (PBE) generalized gradient approximation (GGA) [1], as implemented in the Quantum-ESPRESSO code [2]. Raw, filtered and analyzed. |
| Data format | To generate the structures, we used typical parameters for USPEX calculations, with which efficiency is known to be very high. The USPEX input file was configured in its variable composition mode to produce Nb$_x$N$_y$ structures with a maximum of 30 atoms in the primitive cell. These conditions were replicated for each pressure conditions. In each case, two relaxation processes were implemented with Quantum-ESPRESSO, the first one with a precision of $4 \times 10^{-6}$ and the second one with a precision of $1 \times 10^{-6}$. |
| Parameters for data collection | During the structure searching, the first generation contained 20 candidate structures is produced randomly, considering that all possible stoichiometries in the bulk were allowed for up to 30 atoms in the primitive cell. In the succeeding generations, each generation contained 20 structures, which were obtained by applying 20% heredity, 20% randomly, 20% softmutacion, 20% transmutation respectively. |
| Description of data collection | Universidad del Magdalena, Santa Marta, Magdalena, Colombia. |
| Data source location | Repository name: Complementary material: Data sets of predicted stable and meta-stable crystalline phase structural of Nb-N system under pressure. Data identification number: 10.17632/26b8njvyc8.3 |
| Data accessibility | Direct URL to data: https://data.mendeley.com/datasets/26b8njvyc8/3 |

Value of the data

- The phases obtained are important to better understand the physical essence of Nb$_x$N$_y$ and its practical engineering applications. Knowing the structure, a large number of properties of a material can be calculated, even before it is synthesized, hence the usefulness or crucial importance of the data present here.
- Niobium nitride have been shown to possess interesting properties [3,5], but these researches have always been conducted under ambient pressure. Whereby the data of different crystal structures of Nb$_x$N$_y$ under environmental conditions and high pressures will lay a foundation for both theoretical and experimental researchers for characterization analysis and further technology evaluation of this compound.
- These data shown that the Nb$_x$N$_y$ can possess multiple stoichiometries and structures under different pressures. Understanding the structure of materials is crucial for understanding their properties and potential applications. Researchers can make use of the data presented to characterize these structures.
- Determination of the crystal structure of most materials at normal conditions could be trivial by experimental techniques. However, at extreme conditions, the same treatment becomes extremely problematic, and computer simulation becomes essential for obtaining structural information. Not only at extreme but also at normal conditions crystal structure prediction is of enormous value and a necessary key step in computational materials discovery.
1. Data description

The data here reported correspond to 532 phases of the Nb-N system at different pressures (135 at 0 GPa, 130 at 30 GPa, 134 at 50 GPa and 135 at 100 GPa), which were performed using evolutionary algorithm methodology implemented in the USPEX [6,8] code in its variable composition mode [9,10]. All these data are included in the files: Individuals_0GPa, Individuals_30GPa, Individuals_50GPa, and Individuals_100GPa of the complementary material.

Some structures mentioned above make up a convex hull for each pressure, which is defined as the Gibbs free energy of formation of the most stable phases at each composition, as seen in equation 1:

$$Y = \Delta G(Nb_xN_y) = \frac{[G(Nb_xN_y) - xG(Nb) - yG(N)]}{(x+y)}$$

(1)

Where, $Y = \Delta G(Nb_xN_y)$ is the formation enthalpy of the $Nb_xN_y$ system, $x$ and $y$ are the number of Nb and N atoms respectively.

Thus, of the 135 structures generated for the pressure 0 GPa, 70 of them are present in the convex hull displayed in the following figure.

The characteristics of the first 10 phases include in the convex hull at 0GPa are listed in Table 1.

The Crystal structures of the firsts nine phases presented in Table 1 are schematically shown in Fig. 2.

For the Case 30 GPa, of the 130 structures generated, 59 of them are present in the convex hull shown in Fig. 3.

In the Table 2 are listed the characteristics of the first 10 structures presented in the convex hull at 30 GPa.
Table 1
Formation enthalpy \( Y \) (eV/atom), Composition ratio \( X \), Symmetry \( S \), Fitness \( F \) (eV/block), Volumes \( V(\text{Å}^3/\text{atom}) \), Enthalpies \( E(\text{eV/atom}) \), and Compositions \( C \) for the first 10 structures include in the convex hull of the Nb-N system at 0 GPa.

| ID  | C   | E     | V     | F     | S | X   | Y     |
|-----|-----|-------|-------|-------|---|-----|-------|
| 71  | \([7\ 8]\) | \(-893.5888\) | 14.4958 | 0.0000 | 1 | 0.533 | \(-0.9929\) |
| 75  | \([0\ 14]\)  | \(-270.1198\) | 14.3751 | 0.0000 | 1 | 1.000 | 0.0000 |
| 89  | \([14\ 3]\)   | \(-1369.2158\) | 18.0875 | 0.0000 | 1 | 0.176 | \(-0.6086\) |
| 97  | \([15\ 0]\)   | \(-1603.9973\) | 22.8193 | 0.0000 | 1 | 0.000 | 0.0000 |
| 113 | \([13\ 6]\)   | \(-1183.5582\) | 16.1519 | 0.0000 | 1 | 0.316 | \(-0.7854\) |
| 121 | \([6\ 9]\)    | \(-804.6286\)  | 14.7112 | 0.0000 | 1 | 0.600 | \(-0.9578\) |
| 123 | \([5\ 10]\)   | \(-715.6656\)  | 13.0397 | 0.0000 | 1 | 0.667 | \(-0.9200\) |
| 125 | \([4\ 11]\)   | \(-626.5662\)  | 18.2131 | 0.0000 | 1 | 0.733 | \(-0.7457\) |
| 132 | \([6\ 5]\)    | \(-958.6407\)  | 14.8818 | 0.0000 | 1 | 0.455 | \(-0.9513\) |
| 66  | \([6\ 13]\)   | \(-692.2129\)  | 10.5334 | 0.0055 | 1 | 0.684 | \(-0.8686\) |

Fig. 2. Crystal structures of first nine phases present in the convex hull at 0 GPa. The blue balls are Nb atoms and the green balls are N atoms.

The following figure shows the crystal structures of the firsts nine phases presented in Table 2.

For 50 GPa, of the 134 structures generated, 82 of them are present in the convex hull shown in Fig. 5. The characteristics of the first 10 structures presented in the convex hull at 50 GPa are listed in Table 3.

The Fig. 6 shows the crystal structures of the firsts nine phases presented in Table 3. For the Case 100 GPa, of the 135 structures generated, 73 of them are present in the convex hull displayed in Fig. 7.

The Table 4 shows the characteristics of the first 10 structures present in the convex hull at 100 GPa.

The Crystal structures of the firsts nine phases presented in Table 4 are schematically shown in Fig. 2.

For each one of the considered pressures, the phases that make up the corresponding convex hull and the structural representation in a POSCAR file format are contained respectively in the files, extended_convex_hull_ZGPa and extended_convex_hull_POSCARS_ZGPa (with \( Z = 0, 30, 50, \) and 100), included in the supplementary material.
Table 2
Formation enthalpy $Y$ (eV/atom), Composition ratio $X$, Symmetry $S$, Fitness $F$ (eV/block), Volumes $V$(Å$^3$/atom), Enthalpies $E$(eV/atom), and Compositions $C$ for the first 10 structures include in the convex hull of the Nb-N system at 30GPa.

| ID  | C     | E      | V      | F       | S | X   | Y     |
|-----|-------|--------|--------|---------|---|-----|-------|
| 32  | [16  5] | $-1287.1755$ | $18.1217$ | $0.0000$ | 1 | 0.238 | $-0.5553$ |
| 75  | [0  9]  | $-270.1825$   | $16.1194$ | $0.0000$ | 1 | 1.000 | $0.0000$ |
| 105 | [24  0] | $-1604.2570$ | $23.0125$ | $0.0000$ | 1 | 0.000 | $0.0000$ |
| 107 | [13  9] | $-1059.3153$ | $14.4932$ | $0.0000$ | 1 | 0.409 | $-0.8161$ |
| 116 | [7  13] | $-738.0236$   | $16.5452$ | $0.0000$ | 1 | 0.650 | $-0.9150$ |
| 112 | [16  5] | $-1287.1669$ | $18.1217$ | $0.0086$ | 1 | 0.238 | $-0.5467$ |
| 95  | [12  5] | $-1212.5120$ | $16.4024$ | $0.0089$ | 1 | 0.294 | $-0.6318$ |
| 81  | [24  0] | $-1604.2386$ | $23.0125$ | $0.0184$ | 1 | 0.000 | $0.0184$ |
| 85  | [12  9] | $-1033.3115$ | $16.8773$ | $0.0234$ | 1 | 0.429 | $-0.8007$ |
| 51  | [24  0] | $-1604.1912$ | $23.0125$ | $0.0658$ | 1 | 0.000 | $0.0658$ |

Fig. 3. The Convex hull diagram of the Nb-N system at 30GPa.

Table 3
Formation enthalpy $Y$ (eV/atom), Composition ratio $X$, Symmetry $S$, Fitness $F$ (eV/block), Volumes $V$(Å$^3$/atom), Enthalpies $E$(eV/atom), and Compositions $C$ for the first 10 structures include in the convex hull of the Nb-N system at 50GPa.

| ID  | C     | E      | V      | F       | S | X   | Y     |
|-----|-------|--------|--------|---------|---|-----|-------|
| 8   | [23  0] | $-1604.0754$ | $22.8215$ | $0.0000$ | 2 | 0.000 | $0.000$  |
| 18  | [9  2]  | $-1362.0233$ | $19.9797$ | $0.0000$ | 8 | 0.182 | $-0.6457$ |
| 69  | [2  13] | $-448.3141$  | $15.0906$ | $0.0000$ | 1 | 0.867 | $-1.0985$ |
| 70  | [0  12] | $-269.2371$  | $7.5067$  | $0.0000$ | 1 | 1.000 | $0.0000$ |
| 90  | [12  11] | $-967.3247$ | $15.3563$ | $0.0000$ | 1 | 0.478 | $-1.6502$ |
| 53  | [8  18] | $-681.2706$  | $12.4209$ | $0.0322$ | 1 | 0.692 | $-1.3140$ |
| 125 | [0  12] | $-269.1999$ | $7.5067$  | $0.0372$ | 1 | 1.000 | $0.0372$ |
| 28  | [23  0] | $-1604.0290$ | $22.8215$ | $0.0465$ | 1 | 0.000 | $0.0465$ |
| 34  | [18  2] | $-1470.8920$ | $21.2585$ | $0.0548$ | 1 | 0.100 | $-0.3004$ |
| 43  | [0  11] | $-269.1667$  | $7.2106$  | $0.0703$ | 1 | 1.000 | $0.0703$ |
**Fig. 4.** Crystal structures of first nine phases present in the convex hull at 30 GPa. The blue balls are Nb atoms and the green balls are N atoms.

**Fig. 5.** The Convex hull diagram of the Nb-N system at 50 GPa.
Fig. 6. Crystal structures of first nine phases present in the convex hull at 50 GPa. The blue balls are Nb atoms and the green balls are N atoms.

Fig. 7. The Convex hull diagram of the Nb-N system at 100 GPa.
Fig. 8. Crystal structures of first nine phases present in the convex hull at 100 GPa. The blue balls are Nb atoms and the green balls are N atoms.

Table 4
Formation enthalpy Y (eV/atom), Composition ratio X, Symmetry S, Fitness F (eV/block), Volumes V(Å³/atom), Enthalpies E(eV/atom), and Compositions C for the first 10 structures included in the convex hull of the Nb-N system at 100 GPa.

| ID | C     | E      | V     | F      | S       | X     | Y     |
|----|-------|--------|-------|--------|---------|-------|-------|
| 26 | [17 10] | −1110.9227 | 17.0387 | 0.0000 | 1       | 0.370 | −1.1849 |
| 28 | [27 0] | −1604.0364 | 22.8210 | 0.0000 | 144     | 0.000 | 0.000 |
| 46 | [8 2] | −1337.8241 | 19.6973 | 0.0000 | 53      | 0.200 | −0.7089 |
| 71 | [2 9] | −513.0993  | 13.4886 | 0.0000 | 1       | 0.818 | −1.0133 |
| 92 | [7 14] | −715.7423  | 17.7711 | 0.0000 | 1       | 0.667 | −1.4432 |
| 108| [13 16] | −869.2586 | 14.2094 | 0.0000 | 1       | 0.552 | −1.5566 |
| 110| [27 1] | −1556.5567 | 21.1000 | 0.0000 | 1       | 0.036 | −0.1848 |
| 127| [1 12] | −372.6535  | 9.3197  | 0.0000 | 1       | 0.923 | −0.5611 |
| 133| [0 9] | −269.4304  | 8.0945  | 0.0000 | 1       | 1.000 | 0.0000 |
| 130| [0 11] | −269.4190  | 8.0942  | 0.0114 | 1       | 1.000 | 0.0114 |

To obtain the POSCAR files, corresponding to the phases here predicted, the procedure described in the Fig. 9 was followed. In the Fig. 9 it is shown the amount of generations used, the number of individuals or phases created, and the operations implemented to generate the new individuals.

2. Experimental design, materials, and methods

Searches for stable and metastable structures of the Nb–N system were performed using USPEX in its variable composition mode, together with Quantum-ESPRESSO (QE) [11,12], to carry out a relaxation calculation. The prediction calculations were done for five generations with 20 individuals each one. These individuals were produced under the following constraints: 40% produced by inheritance, 20% produced by random, 20% produced by soft mutation and 20% produced by transmutation, each individual can have a maximum of 30 atoms and a minimum of 1. The process for predict stable and metastable structures of the Nb–N system is described in the following figure.
To perform the process schematically described in the Fig. 9, the input file, INPUT.txt, it must configure and create a folder called Specific. All the parameter to perform the calculation, such as the type of atoms, species, symmetries to explore, pressure, number of individuals (structures that USPEX will predict), number of generations, and any other characteristics that structurally affect the phases that will be generated, are configured in the file INPUT.txt. In addition, in this input file, the computational suite is selected to relax the created structures and the instruction to execute it.

**Declaration of Competing Interest**

The authors declare that they have no known competing financial interests or personal relationships, which have, or could be perceived to have, influenced the work reported in this article.

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**Supplementary materials**

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.dib.2020.106054.

**References**

[1] J.P. Perdew, K. Burke, M. Ernzerhof, Generalized gradient approximation made simple, Phys. Rev. Lett. 77 (18) (1996) 3865, doi:10.1103/physrevlett.77.3865.

[2] G. Kresse, J. Furthmüller, Efficient iterative schemes for ab initio total-energy calculations using a plane-wave basis set, Phys. Rev. B 54 (1996) 11169–11186, doi:10.1103/PhysRevB.54.11169.

[3] L. Toth (Ed), Transition metal carbides and nitrides, Elsevier (2014).
[4] E.K. Storms, The Refractory Carbides, Elsevier, 2016.

[5] G.F. Hardy, J.K. Hulm, The superconductivity of some transition metal compounds, Phys. Rev. 93 (5) (1954) 1004, doi:10.1103/PhysRev.93.1004.

[6] A.R. Oganov, C.W. Glass, Crystal structure prediction using ab initio evolutionary techniques: principles and applications, J Chem Phys 124 (24) (2006) 244704, doi:10.1063/1.2210932.

[7] A.R. Oganov, H. Stokes, M. Valle, How evolutionary crystal structure prediction works - and why, Acc. Chem. Res. 44 (3) (2011) 227–237, doi:10.1021/ar1001318.

[8] A.O. Lyakhov, A.R. Oganov, H. Stokes, M. Valle, Crystal structure prediction using evolutionary approach, in: A.R. Oganov (Ed.), Modern Methods of Crystal Structure Prediction, Wiley-VCH, Berlin, 2010, doi:10.1002/9783527632831.ch7.

[9] A.R. Oganov, Y. Ma, A.O. Lyakhov, M. Valle, C. Gatti, Evolutionary crystal structure prediction as a method for the discovery of minerals and materials, Rev. Mineral. Geochem. 71 (2010) 271–298, doi:10.2138/rmg.2010.71.13.

[10] P. Giannozzi, S. Baroni, N. Bonini, M. Calandra, R. Car, C. Cavazzoni, D. Ceresoli, G.L. Chiarotti, M. Cococcioni, I. Dabo, A. Dal Corso, S. Fabris, G. Fratesi, S. de Gironcoli, R. Gebauer, U. Gerstmann, C. Gougoussis, A. Kokalj, M. Lazzeri, L. Martin-Samos, N. Marzari, F. Mauri, R. Mazzarello, S. Paolini, A. Pasquarello, L. Paulatto, C. Scandolo, S. Scandolo, G. Sclauzero, A.P. Seitsonen, A. Smogunov, P. Umari, R.M. Wentzcovitch, J. Phys. 21 (2009) 395502, doi:10.1088/0953-8984/21/39/395502.

[11] P. Giannozzi, O. Andreussi, T. Brumme, O. Bunau, M. Buongiorno Nardelli, M. Calandra, R. Car, C. Cavazzoni, D. Ceresoli, M. Cococcioni, N. Colonna, I. Carnimeo, A. Dal Corso, S. de Gironcoli, P. Delugas, R.A. DiStasio Jr, A. Ferrari, A. Floris, G. Fratesi, G. Fugallo, R. Gebauer, U. Gerstmann, F. Giustino, T. Gorni, J. Jia, M. Kawamura, H.-Y. Ko, A. Kokalj, E. Küçükbenli, M. Lazzeri, M. Marsili, N. Marzari, F. Mauri, N.L. Nguyen, H.-V. Nguyen, A. Otero-de-la-Roza, L. Paulatto, S. Ponce, D. Roccia, R. Sabatini, B. Santra, M. Schlipf, A.P. Seitsonen, A. Smogunov, I. Timrov, T. Thonhauser, P. Umari, N. Vast, X. Wu and S. Baroni, Journal of physics: condensed matter, 29 (2017), 465901, doi:10.1088/1361-648X/aa8f79.