Insight into the physical properties of two niobium based compounds Nb$_3$Be and Nb$_3$Be$_2$ via first principles calculation

Md. Zahidur Rahaman$^1$

Department of Physics
Pabna University of Science and Technology, Pabna-6600, Bangladesh
Bangladesh University of Engineering and Technology, Dhaka, Bangladesh
zahidur.physics@gmail.com

Md. Lokman Ali$^2$

Department of Physics
Pabna University of Science and Technology, Pabna-6600, Bangladesh
lokman.cu12@gmail.com

(28 August, 2017)

Abstract

We investigate the structural, electronic, mechanical and elastic properties of two niobium based intermetallic compounds Nb$_3$Be and Nb$_3$Be$_2$ by using the DFT based theoretical method. A good agreement is found among the structural parameters of both the phases with experimentally evaluated parameters. For both the phases metallic conductivity is observed while Nb$_3$Be phase is more conducting than that of Nb$_3$Be$_2$ phase. Evaluated DOS at Fermi level indicates that Nb$_3$Be$_2$ phase is electrically more stable than Nb$_3$Be phase. For both phases Nb-4d states is mostly responsible for metallic conductivity. The study of total charge density and Mulliken atomic population reveal the existence of covalent, metallic and ionic bonds in both intermetallics. Both the phases are mechanically stable in nature while Nb$_3$Be phase is more ductile than Nb$_3$Be$_2$ phase. The study of Vickers hardness exhibits that Nb$_3$Be$_2$ phase is harder than that of Nb$_3$Be. Both compounds are anisotropic in nature while Nb$_3$Be phase possesses large anisotropic characteristics than that of Nb$_3$Be$_2$ phase. The Debye temperature of both the compounds are also calculated and discussed.

Keywords: Crystal structure, Electronic properties, Mechanical properties, Debye temperature.
I. Introduction

A-15 structured materials have gained huge interest in the research community of solid state physics as well as material science for more than five decades due to their many attractive physical properties. Most of the compound in this family exhibits superconductivity; some of them show high superconducting critical temperature. Many of them possess unusual elastic and electrical properties. Many compounds of A-15 family possess good corrosion resistance, low density and high melting point. Not only in superconductor industry but also these intermetallics have a number of applications in chemical industries, aerospace industry, aircraft, biomedical instrumentations and hydrogen storage systems.

In 1931 Hartman et al. first observed the cubic A-15 structure [1]. A-15 phases possess the A₃B type composition, where A = any transition metal and B = element from right side of the periodic table [2-4]. Among the A₃B type compounds, much interest has been drawn those intermetallics which shows superconductivity. For example, vanadium gallium (V₃Ga) is often used in superconducting electromagnet [5]. The critical temperature and upper critical field of V₃Ga is 14.2 K and 19 Tesla respectively [6].

However, niobium (Nb) constitutes a number of superconductors with a wide range of $T_c$, such as Nb₃Sb (0.2 K), Nb₃In (9.2 K), Nb₃Bi (3 K), Nb₃Al (18.8 K), Nb₃Ge (23.6 K), Nb₃Sn (18.9 K), Nb₃Ga (20.2 K) [7]. All these compounds belong to Cr₃Si structure type [8-14]. Superconductivity in niobium beryllide (Nb₃Be) was first observed by Tuleushev et al. in 2003 [15]. They used thermal treatment of the amorphous film system to synthesize Nb₃Be. They obtained X-ray structural data to identify the structure of Nb₃Be. They also determined the superconducting critical temperature ($T_c$ ) of Nb₃Be as 10.0 K. However, except the structural and superconducting properties of Nb₃Be there is no more information available in literature. On the other hand, Nb₃Be₂ phase possesses the same reactant element as Nb₃Be phase though their chemical composition is quite different. So it is very interesting to study and compare the physical properties of these two different phases of Nb-Be system. Nb₃Be₂ phase was first synthesized by Zalkin et al. in 1960 by using X-ray powder diffraction technique [16]. In their study, they found that in Nb₃Be₂ phase the powder pattern indicates the presence of a fcc unit cell with
lattice constant 10.94 Å. Though they concluded the selected phase as an impurity or an additional phase in Nb-Be system. However, except the structural determination no further investigation has been done on Nb$_3$Be$_2$ phase up to now.

Therefore, in this present work we aim to study the detailed physical properties of Nb$_3$Be and Nb$_3$Be$_2$ phases by theoretical means. A thorough comparison among the obtained physical properties of these two phases have also been represented and discussed from the theoretical view point.

II. Method of computation

All theoretical calculations in the present work were performed by using UPPW (Ultra-soft Pseudopotential Plane Wave) method based on DFT (Density Functional Theory) implemented within CASTEP (Cambridge Serial Total Energy Package) code [17]. GGA (Generalized Gradient Approximation) was used to describe the exchange-correlation functional parametrized by Perdew-Burke-Ernzerhof (PBE) [18-21]. For pseudo atomic calculation Nb-4s$^2$ 4p$^6$ 4d$^4$ 5s$^1$ and Be-2s$^2$ for both the compounds were taken as valence electron. For constructing the k-point meshes for the sake of Brillouin zone sampling Monkhorst-Pack scheme [22] was used. For converging the total energy 8×8×8 grids with 400 eV cutoff energy for Nb$_3$Be and 8×8×8 grids with 350 eV cutoff energy for Nb$_3$Be$_2$ were set. The full geometry optimization of both the compounds was performed within BFGS (Brodyden-Fletcher-Goldfarb-Shanno) scheme [23]. The elastic stiffness constants of Nb$_3$Be and Nb$_3$Be$_2$ intermetallics were computed by using the stress-strain method [24]. The maximum ionic displacement was fixed to 2.0 × 10$^{-4}$ Å.

III. Results and discussion

A. Structural Properties

A-15 structured superconductor Nb$_3$Be possesses cubic crystal structure with PM-3N (223) space group [15] whereas Nb$_3$Be$_2$ phase possesses tetragonal crystal structure with
space group $P4/MBM$ (127) [16]. Nb$_3$Be has eight atoms per unit cell with two formula units whereas Nb$_3$Be$_2$ phase has ten atoms per unit cell with two formula units. The detailed fractional coordinates of Nb$_3$Be$_2$ can be found elsewhere [16]. The fully relaxed crystal structures of both the compounds are illustrated in Fig. 1. The computed lattice constants $a_0$ and $c_0$, cell volume $V_0$ and bulk modulus $B_0$ of both the phases are listed in Table 1 along with the experimental values. From Table 1 it can be noticed that the computed structural parameters in this study are in good agreement with the experimentally evaluated parameters. Theoretically evaluated lattice constant shows minor deviation with experimental value bearing the reliability of this present study.

**B. Single and Polycrystalline Elastic Properties**

The cubic and tetragonal solids have three ($C_{11}$, $C_{12}$ and $C_{44}$) and six ($C_{11}$, $C_{12}$, $C_{13}$, $C_{33}$, $C_{44}$ and $C_{66}$) independent elastic constants respectively. These elastic constants can be achieved by computing the total energy as a function of strain [25]. The detailed of these calculations are explained elsewhere [26, 27]. The obtained elastic constants of both the phases are recorded in Table 2. There is no previous data available in literature about the elastic constants of these two phases. Hence, this present study will be a valuable source of reference for future experimental work. As shown in Table 2, the value of $C_{33}$ is larger than that of $C_{11}$ for Nb$_3$Be$_2$ implying that the incompressibility toward [001] direction is stronger than [100] direction [28]. We also notice that $C_{44}$ is smaller than $C_{66}$ indicating that [100](010) shear is harder than [100](001) shear for Nb$_3$Be$_2$ [28]. It can be noted that almost all the elastic constants of Nb$_3$Be are slightly smaller than that of Nb$_3$Be$_2$ phase implying the weaker shear resistance and incompressibility of Nb$_3$Be compared with Nb$_3$Be$_2$. The calculated elastic constants of both the phases are also compared with Nb$_3$Ga as shown in Table 2.

For being mechanically stable the strain energy of a crystal must be positive for homogeneous elastic deformation of the crystal [28]. The Born stability criteria for tetragonal solids are given below.

$$C_{11} > 0, \ C_{33} > 0, \ C_{66} > 0, \ C_{44} > 0, \ C_{11} + C_{33} - 2C_{13} > 0, \ C_{11} - C_{12} > 0, \ 2(C_{11} + C_{33}) - 5C_{12} > 0 \text{, and } C_{11} - C_{33} - 2C_{13} > 0.$$
For cubic crystal there are only three elastic constants and hence the stability criteria is written as,

\[ C_{11} > 0, \; C_{44} > 0, \; C_{11} - C_{12} > 0 \; \text{and} \; C_{11} + 2C_{12} > 0 \]

Evidently, the above two phases of Nb are mechanically stable in nature as their computed elastic constant data satisfy the respective stability criteria as shown in Table 2. The elastic moduli of polycrystalline compounds can be achieved from the single crystal elastic constants data by using VRH (Voigt-Reuss-Hill) scheme [29]. This scheme provides reasonably satisfactory data of elastic constants which has been validated experimentally. For tetragonal solids the bulk and shear modulus in this approximation are given as follows:

\[
B_V = \frac{2C_{11} + 2C_{12} + C_{33} + 4C_{13}}{9} \tag{1}
\]

\[
B_R = \frac{C^2}{M} \tag{2}
\]

\[
G_V = \frac{M + 3C_{11} - 3C_{12} + 12C_{44} + 6C_{66}}{30} \tag{3}
\]

\[
G_R = \frac{15}{\left[\frac{18B_V}{C^2} + \frac{6}{(C_{11} - C_{12})} + \frac{6}{C_{44}} + \frac{3}{C_{66}}\right]} \tag{4}
\]

Where,

\[
M = C_{11} + C_{12} + 2C_{33} - 4C_{13}
\]

And

\[
C^2 = (C_{11} + C_{12})C_{33} - 2C_{13}^2
\]

For cubic crystal we get,

\[
B_v = B_R = \frac{(C_{11} + 2C_{12})}{3} \tag{5}
\]

\[
G_v = \frac{(C_{11} - C_{12} + 3C_{44})}{5} \tag{6}
\]

\[
G_R = \frac{5C_{44}(C_{11} - C_{12})}{[4C_{44} + 3(C_{11} - C_{12})]} \tag{7}
\]
Now, the value of $B$ and $G$ can be obtained as follows,

$$B = \frac{1}{2} (B_R + B_v)$$ \hspace{1cm} (8)

$$G = \frac{1}{2} (G_v + G_R)$$ \hspace{1cm} (9)

The Poisson’s ratio, $\nu$ and Young’s modulus, $E$ can be estimated by using the following formulas,

$$\nu = \frac{3B - 2G}{2(3B + G)}$$ \hspace{1cm} (10)

$$E = \frac{9GB}{3B + G}$$ \hspace{1cm} (11)

The estimated polycrystalline elastic moduli are tabulated in Table 3. The calculated elastic moduli of both the phases are also compared with Nb$_3$Ga. As shown in Table 3 the bulk modulus of Nb$_3$Be$_2$ phase is slightly larger than the Nb$_3$Be phase implying the stronger resistance to change in volume of Nb$_3$Be$_2$ phase under external pressure [30]. The shear modulus of Nb$_3$Be$_2$ phase is comparatively large than that of Nb$_3$Be phase indicating strong shear resistance and strong covalent bond in Nb$_3$Be$_2$ phase [31]. The ratio between axial strain and uniaxial stress is generally defined as the Young’s modulus, which provides information about the stiffness of solids [32]. Comparatively large value of Young’s modulus of Nb$_3$Be$_2$ phase indicates that Nb$_3$Be$_2$ is stiffer than the Nb$_3$Be phase.

In order to identify the intrinsic ductility of solids the Poisson’s ratio is a useful index. The higher the Poisson’s ratio, the more ductile the material is. According to the value of Poisson’s ratio $\nu$ (Table 3) both the phases are ductile and ductility of Nb$_3$Be phase is better than Nb$_3$Be$_2$ phase. The Poisson’s ratio is also used to predict the bonding force exist in a solid. As shown in Table 3 both the phases exhibit central force characteristics as the value of $\nu$ from 0.25 to 0.50 indicates the existence of central force in a solid [33]. Another empirical criterion to judge the brittleness and ductility of solids is Pugh ratio (the ratio between the bulk modulus $B$ and shear modulus $G$, $B/G$) [32]. As shown in Table 3 both the compounds exhibit ductile manner as $B/G > 1.75$. Though, Nb$_3$Be phase is more ductile than Nb$_3$Be$_2$ phase. This result accords well with that predicted form the value of Poisson’s ratio. Cauchy pressure is another useful
index to explain the angular character of atomic bonding in solids [34]. For tetragonal phase the Cauchy pressures \((C_{13} - C_{44})\) and \((C_{12} - C_{66})\) as well as for cubic phase the Cauchy pressure \((C_{12} - C_{44})\) are evaluated and listed in Table 3. Obviously the positive value of Cauchy pressure for both the compounds demonstrates the ductile manner [35] consistent with above prediction.

The Vickers hardness is a very popular index to get information about the hardness of a material. In this study we have used a very simple potential formula developed by Chen et al [36] for calculating the hardness of \(\text{Nb}_3\text{Be}\) and \(\text{Nb}_3\text{Be}_2\) phases given as follows,

\[
H_v = 2 \left( K^2 G \right)^{0.585} - 3
\]  \hspace{1cm} (12)

Where, \(K\) is defined as the ratio between shear modulus and bulk modulus. Evaluated values of \(H_v\) using eq. 12 for both phases are listed in Table 3. Obviously, the computed values represent similar trend as predicted above by Young’s modulus that \(\text{Nb}_3\text{Be}_2\) phase is harder than that of \(\text{Nb}_3\text{Be}\).

The anisotropic characteristics of a tetragonal crystal can be computed by the following equation [37],

\[
A^U = \frac{5G_V}{G_R} + \frac{B_V}{B_R} - 6
\]  \hspace{1cm} (13)

For cubic crystal the evaluated value of bulk modulus is same according to Voigt and Reuss approximation and hence Eq. 13 can be simplified as,

\[
A^U = 5 \left( \frac{G_V}{G_R} - 1 \right)
\]  \hspace{1cm} (14)

The evaluated values of \(A^U\) by using Eq. 13 and Eq. 14 for tetragonal \(\text{Nb}_3\text{Be}_2\) and cubic \(\text{Nb}_3\text{Be}\) phase are tabulated in Table 3. For completely isotropic material \(A^U = 0\), and deviation from zero indicates the degree of anisotropy. As shown in Table 3 both the phases are anisotropic in nature and \(\text{Nb}_3\text{Be}\) phase possesses large anisotropic characteristics than that of \(\text{Nb}_3\text{Be}_2\) phase.
C. Electronic Properties and Chemical Bonding

The electronic properties of cubic Nb₃Be and tetragonal Nb₃Be₂ phase have been investigated through the calculation of band structure, partial and total density of states and total electron (charge) density. The band structures of both the Nb-phase are illustrated in Fig. 2. Evidently, at Fermi level the valence and conduction bands are overlapped implying the metallic nature of both the phases. Though the superconducting properties of Nb₃Be have been investigated previously, the superconducting properties of Nb₃Be₂ phase are still unexplored. The metallic nature of Nb₃Be₂ phase implies that this phase may also possess superconducting characteristics [38].

The total and partial density of states of Nb₃Be and Nb₃Be₂ phases are illustrated in Fig. 3. From -8 eV to 0 eV (Fermi level) the prevalent feature of hybridization is noticed for Nb-4d and Be-2s states for both the intermetallics with some contribution of Nb-5s and Nb-4p states. Nb-4d states contribute the most to constitute the valence band of both phases. In conduction band most of the contribution comes from Nb-4d states. Though, some of the contribution comes from Nb-4p states. For both the compounds approximately null contribution is observed for Be-2s states in conduction band. However the contribution of Nb-4d states is most at Fermi level. Nb metal is responsible for the metallic nature of both the phases. The computed density of states at Fermi level is 13.82 states per eV per unit cell for Nb₃Be phase and 3.81 states per eV per unit cell for Nb₃Be₂ phase. Therefore, Nb₃Be phase is more conducting than that of Nb₃Be₂ phase. For metallic system, the electronic stability depends upon the value of DOS at Fermi level. Metal having lower value of \( N (E_F) \) shows more stability than those having higher value of \( N (E_F) \) [42]. According to this condition Nb₃Be₂ phase is electrically more stable than Nb₃Be phase.

For analyzing the bonding characteristics of Nb₃Be and Nb₃Be₂ phases Mulliken atomic populations [39] have been calculated. The data of atomic populations is very handful to understand the chemical bonding characteristics of materials. A null value of bond population implies the ionic nature of that particular bond whereas high value indicates the increasing level of covalency [40]. The estimated bond populations of both
the phases are listed in Table 4. It is evident from Table 4 that the bond populations of both the compounds are positive and greater than zero implying the existence of covalent bonds in both phases. For both the phases Be atom carries the negative charges indicating the transfer of electron from Nb to Be atom. Transferring of charge from one atom to another precisely indicates the existence of ionic bonds in both compounds. The corresponding bond lengths of both phases are also shown in Table 4.

For further understanding the bonding nature in Nb$_3$Be and Nb$_3$Be$_2$ phases the total charge (electron) density is calculated along (001) plane as illustrated in Fig. 4. A scale is shown at the right side of both plots indicating the intensity of charge density. For both the compounds there are no overlapping of electron distribution appeared. This result represents the existence of ionic bond in Nb$_3$Be and Nb$_3$Be$_2$. But ionic nature is the result of metallic character [41] indicating the existence of metallic bonds in both phases. Therefore we can conclude that all the covalent, ionic and metallic bonds are formed in Nb$_3$Be and Nb$_3$Be$_2$ compounds and contribute equally for the stability of both the phases.

D. Debye Temperature

The Debye temperature is the temperature which is associated with the highest normal mode of oscillation of a crystal [43]. It is associated directly or indirectly with many significant thermal characteristics of crystals for example specific heat, melting point, thermal expansion etc. So it is reasonable to determine the Debye temperature of Nb$_3$Be and Nb$_3$Be$_2$ phases. However, there are various procedures and estimations available for computing the value of $\Theta_D$. In this present study we have employed the computed elastic constants to evaluate the Debye temperature of Nb$_3$Be and Nb$_3$Be$_2$ intermetallics. The average wave velocity ($V_m$) of a solid is formulated as,

$$v_m = \left[ \frac{1}{3} \left( \frac{2}{v_l^3} + \frac{1}{v_t^3} \right) \right]^{-\frac{1}{3}}$$  \hspace{1cm} (15)
Where, $V_l$ and $V_t$ are longitudinal and transverse wave velocity respectively can be obtained as follows,

$$v_l = \left( \frac{3B + 4G}{3\rho} \right)^{\frac{1}{2}}$$  \hspace{1cm} (16)

And

$$v_t = \left( \frac{G}{\rho} \right)^{\frac{1}{2}}$$  \hspace{1cm} (17)

Now, the Debye temperature ($\Theta_D$) can be computed as follows [44],

$$\Theta_D = \frac{h}{k_B} \left( \frac{3N}{4\pi V} \right)^{\frac{1}{3}} \times v_m$$  \hspace{1cm} (18)

Where, $k_B$ is the Boltzmann constant and $h$ is the Planck constant. The computed values of $V_l$, $V_t$, $V_m$ and $\Theta_D$ for Nb$_3$Be and Nb$_3$Be$_2$ phases are listed in Table 5. As shown in Table 5 the Debye temperature of Nb$_3$Be$_2$ phase is larger than that of Nb$_3$Be phase. These values imply that for a single normal vibration of Nb$_3$Be crystal the highest temperature can be achieved as 368.36 K and for Nb$_3$Be$_2$ crystal the highest temperature can be achieved as 450.91 K.

**IV. Conclusions**

In summary, the detailed physical properties including structural, mechanical and electronic properties of two Nb-based intermetallic compounds Nb$_3$Be and Nb$_3$Be$_2$ have been explored by using theoretical means. A good agreement is found among the structural parameters of both the phases with experimentally evaluated parameters. For both the phases metallic conductivity is observed while Nb$_3$Be phase is more conducting than that of Nb$_3$Be$_2$ phase. Evaluated DOS at Fermi level indicates that Nb$_3$Be$_2$ phase is electrically more stable than Nb$_3$Be phase. For both phases Nb-4d states is mostly responsible for metallic conductivity with minor contribution of other constituent orbitals. The study of total charge density and Mulliken atomic population reveal the existence of covalent,
metallic and ionic bonds in both intermetallics. The metallic nature of Nb$_3$Be$_2$ phase implies that this phase may also possess superconducting characteristics. The study of elastic constants reveals that both intermetallics are mechanically stable in nature while Nb$_3$Be phase is more ductile than Nb$_3$Be$_2$ phase. Hence fabrication of Nb$_3$Be will be easier than Nb$_3$Be$_2$. The study of Vickers hardness exhibits that Nb$_3$Be$_2$ phase is harder than that of Nb$_3$Be. Both compounds are anisotropic in nature while Nb$_3$Be phase possesses large anisotropic characteristics than that of Nb$_3$Be$_2$ phase. The Debye temperature of Nb$_3$Be is calculated to be 368.36 K and for Nb$_3$Be$_2$ phase 450.91 K. These values imply that for a single normal vibration of Nb$_3$Be crystal the highest temperature can be achieved as 368.36 K and for Nb$_3$Be$_2$ crystal the highest temperature can be achieved as 450.91 K. We hope the predicted physical properties of these two compounds will motivate for technological application of these compounds and also inspire other researcher to conduct detailed experimental research on these interesting materials in future.

1. H. Hartman, F. Ebert, O. Bretschneider, Z. Anorg. Allg. Chem. 198 (1931) 116.
2. M. D. Banus, T. B. Reed, H. C. Gatos, M. C. Lavine, J. A. Kafalas, J. Phys. Chem. Solids 23 (1962) 971.
3. D. H. Killpatrick, J. Phys. Chem. Solids 25 (1964) 1213.
4. Y. Tarutani, U. Kawabe, Mater. Res. Bull. 13 (1978) 469.
5. https://en.wikipedia.org/wiki/Vanadium-gallium
6. Decker, D.L.Laquer, H.L.(1969), Magnetization Studies on Superconducting Vanadium Gallium (PDF), doi:10.1063/1.1658081
7. Sundareswari, M., Swaminathan Ramasubramanian, and Mathrubutham Rajagopalan. "Elastic and thermodynamical properties of A15 Nb$_3$X (X= Al, Ga, In, Sn and Sb) compounds—First principles DFT study." Solid State Communications 150.41 (2010): 2057-2060.
8. E.A. Wood, V.B. Compton, B.T. Matthias, E. Corenzwit, Acta Crystallogr. 11(1958) 604.
9. P.A. Beck (Ed.), Electronic Structure and Alloy Chemistry of the Transition Elements, Interscience Publishers, New York, 1963.

10. N.V. Nevit, in: J.H. Westbrook (Ed.), Intermetallics Compounds, R.E. Krieger Publishing Co., Huntington, NY, 1977.

11. M.D. Banus, T.B. Reed, H.C. Gatos, M.C. Lavine, J.A. Kafalos, J. Phys. Chem. Solids 23 (1962) 971.

12. D.H. Killpatrick, J. Phys. Chem. Solids 25 (1964) 1213.

13. Y. Tarutani, U. Kawabe, Mater. Res. Bull. 13 (1978) 469.

14. R. Fluikiger, H. Kupfer, J.L. Jorda, J. Muller, IEEE Trans. Magn. 23 (1987) 980.

15. Tuleushev, A. Zh, V. N. Volodin, and Yu Zh Tuleushev. "Novel superconducting niobium beryllide Nb\textsubscript{3}Be with A15 structure." JETP Letters 78.7 (2003): 440-442.

16. Zalkin, A., D. E. Sands, and O. H. Krikorian. "Crystal structure of Nb\textsubscript{3}Be\textsubscript{2}." Acta Crystallographica 13.2 (1960): 160-160.

17. Materials Studio CASTEP manual_Accelrys, 2010. Pp. 261–262.

18. S.J. Clark, M.D. Segall, C.J. Pickard, P.J. Hasnip, M.J. Probert, K. Refson, M.C. Payne, Z.Kristallogr. 220 (2005) 567–570.

19. P. Hohenberg, W. Kohn, Phys. Rev. 136 (1964) B864–B871.

20. J.P. Perdew, A. Ruzsinszky, G.I. Csonka, O.A. Vydrov, G.E. Scuseria, L.A. Constantin, X. Zhou, K. burke, Phys. Rev. Lett. 100 (2008) 136406–136409.

21. J.P. Perdew, A. Ruzsinszky, G.I. Csonka, O.A. Vydrov, G.E. Scuseria, L.A. Constantin, X. Zhou, K. Burke, Phys. Rev. Lett. 100 (2008) 136406.

22. H. J. Monkhorst and J. D. Pack, Phys. Rev. B 13, 5188 (1976).

23. B. G. Pfommer, M. Cote, S. G. Louie, and M. L. Cohen, J. Comput. Phys. 131, 233 (1997).

24. J. Kang, E.C. Lee, K.J. Chang, Phys. Rev. B 68 (2003) 054106.

25. L. Fast, J.Wills, B. Johansson, O. Eriksson, Phys. Rev. B 51 (1995) 17431.
26. O. Beckstein, J. Klepeis, G. Hart, O. Pankratov, Phys. Rev. B 63 (2001).

27. B.Y. Tang, N. Wang, W.Y. Yu, X.Q. Zeng, W.J. Ding, Acta Mater. 56 (2008) 3353-3357.

28. Wu, Dong-Hai, et al. "First-principles study of structural stability and elastic properties of MgPd$_3$ and its hydride." Journal of Magnesium and Alloys 2.2 (2014): 165-174.

29. Z.J.Wu, E.J. Zhao, H.P. Xiang, X.F. Hao, X.J. Liu, J. Meng, Phys. Rev. B 76 (2007) 054115.

30. L. Fast, J.Wills, B. Johansson, O. Eriksson, Phys. Rev. B 51 (1995) 17431.

31. Z. Sun, S. Li, R. Ahuja, J.M. Schneider, Solid State Commun. 129 (2004) 589e592.

32. S. Pugh, Philos. Mag. 45 (1954) 823e843.

33. P. Ravindran, L. Fast, P. Korzhavyi, B. Johansson, J. Wills, O. Eriksson, J. Appl. Phys. 84 (1998) 4891.

34. D. Pettifor, Mater. Sci. Technol. 8 (1992) 345e349.

35. D. Suetin, I. Shein, A. Ivanovskii, Solid State Sci. 12 (2010) 814e817.

36. X.Q. Chen, H. Niu, D. Li and Y. Li, Intermetallics 19 (2011) p.1275.

37. S. I. Ranganathan and M. Ostoja-Starzewski, Phys. Rev. Lett. 101, 055504 (2008).

38. Rahaman, Md Zahidur, and Md Atikur Rahman. "Novel Laves phase superconductor NbBe$_2$: A theoretical investigation." Computational Condensed Matter 8 (2016): 7-13.

39. R.S. Mulliken, J. Chem. Phys. 23 (1955) p.1833.

40. Segall, M. D.; Shah, R.; Pickard, C. J.; Payne, M. C. Phys. Rev. B , 54, 16317-16320 (1996).

41. R.P. Singh, Journal of Magnesium and Alloys 2 (2014) 349-356.

42. M.X. Zeng, R.N. Wang, B.Y. Tang, L.M. Peng, W.J. Ding, Model. Simul. Mater. Sci. Eng. 20 (2012) 035018.
43. Rahaman, Md Zahidur, and Md Atikur Rahman. "ThCr$_2$Si$_2$-type Ru-based superconductors LaRu$_2$M$_2$ (M= P and As): An ab-initio investigation." *Journal of Alloys and Compounds* 695 (2017): 2827-2834.

44. S. Aydin, M. Simsek, Phys. Rev. B: Condens. Matter 80 (2009) 134107.

45. Tian, Wenyan, and Haichuan Chen. "Theoretical investigation of the mechanical and thermodynamics properties of Nb$_3$Ga superconductor under pressure." *Journal of Alloys and Compounds* 648 (2015): 229-236.

46. Sundareswari, M., Swaminathan Ramasubramanian, and Mathrubutham Rajagopalan. "Elastic and thermodynamical properties of A15 Nb$_3$X (X= Al, Ga, In, Sn and Sb) compounds—First principles DFT study." *Solid State Communications* 150.41-42 (2010): 2057-2060.
Figure 1: The crystal structure of (a) Nb$_3$Be and (b) Nb$_3$Be$_2$.

Figure 2: The band structure of (a) Nb$_3$Be and (b) Nb$_3$Be$_2$ phase.
Figure 3: Total and partial DOS of (a) Nb$_3$Be$_2$ and (b) Nb$_3$Be intermetallics.

Figure 4: Total charge density on (001) plane of (a) Nb$_3$Be and (b) Nb$_3$Be$_2$ intermetallics.
Table 1: Unit cell parameters of Nb$_3$Be and Nb$_3$Be$_2$ intermetallics.

| Properties | Nb$_3$Be | Expt. [15] | Nb$_3$Be$_2$ | Expt. [16] |
|------------|----------|------------|--------------|------------|
| $a_0$ (Å)  | 5.070    | 5.187      | 6.533        | 6.490      |
| $c_0$ (Å)  | -        | -          | 3.364        | 3.350      |
| $c_0/a_0$  | -        | -          | 0.514        | 0.516      |
| $V_0$ (Å$^3$) | 130.32 | 139.55     | 143.57       | 141.10     |
| $B_0$ (GPa) | 155.42  | -          | 162.23       | -          |

Table 2: The computed elastic constants $C_{ij}$ (in GPa) of Nb$_3$Be and Nb$_3$Be$_2$ phases.

| Compounds | $C_{11}$ | $C_{12}$ | $C_{13}$ | $C_{33}$ | $C_{44}$ | $C_{66}$ |
|-----------|----------|----------|----------|----------|----------|----------|
| Nb$_3$Be  | 275.17   | 89.92    | -        | -        | 40.99    | -        |
| Nb$_3$Be$_2$ | 264.46 | 91.07    | 108.62   | 250.13   | 69.88    | 81.62    |
| Nb$_3$Ga  | 245.50$^a$, 305.41$^b$ | 123.60$^a$, 104.90$^b$ | -        | -        | 39.50$^a$, 48.78$^b$ | -        |

$^a$Ref. 45; $^b$Ref. 46
**Table 3:** Computed bulk modulus $B$ (GPa), shear modulus $G$ (GPa), Young’s modulus $E$ (GPa), $B/G$ values, Poisson’s ratio $\nu$, Cauchy pressures $(C_{12} - C_{66})$, $(C_{13} - C_{44})$ and $(C_{12} - C_{44})$ elastic anisotropy $A^U$ and Vickers hardness $H_v$ (GPa) of Nb$_3$Be and Nb$_3$Be$_2$ phases.

| Compounds | $B$  | $G$  | $E$  | $B/G$ | $\nu$ | $(C_{12} - C_{66})$ | $(C_{13} - C_{44})$ | $(C_{12} - C_{44})$ | $A^U$  | $H_v$  |
|-----------|------|------|------|-------|-------|-------------------|-------------------|-------------------|-------|-------|
| Nb$_3$Be  | 151.67 | 57.19 | 152.41 | 2.65  | 0.33  | -                 | -                 | -                 | 48.93 | 0.84  | 3.81  |
| Nb$_3$Be$_2$ | 155.07 | 74.59 | 192.84 | 2.07  | 0.29  | 9.45             | 38.74             | -                 | 0.14  | 7.58  |
| Nb$_3$Ga  | 164.30$^a$ | 47.0$^a$ | 128.80$^a$ | 3.49$^a$ | 0.36$^a$ | -                 | -                 | -                 | 0.22$^a$ | 3.30$^a$ |       |
|           | 169.97$^b$ | 65.49$^b$ | 174.11$^b$ | -     | 0.30$^b$ | -                 | -                 | -                 | 55.31$^b$ |       |       |

$^a$Ref. 45; $^b$Ref. 46

**Table 4:** Mulliken atomic populations of cubic Nb$_3$Be and tetragonal Nb$_3$Be$_2$ phase.

| Compounds | Species | s | p | d | Total | Charge | Bond     | Population | Length (Å) |
|-----------|---------|---|---|---|-------|--------|----------|------------|------------|
| Nb$_3$Be  | Nb      | 2.19 | 6.60 | 4.13 | 12.92 | 0.08   | Nb-Nb    | 0.48       | 2.5350     |
|           | Be      | 0.54 | 1.69 | 0.00 | 2.23  | -0.23  | Be-Nb    | 0.37       | 2.8343     |
| Nb$_3$Be$_2$ | Nb    | 2.29 | 6.66 | 4.03 | 12.97 | 0.03   | Be-Be    | 0.44       | 2.0806     |
|           | Be      | 0.56 | 1.90 | 0.00 | 2.46  | -0.46  | Be-Nb(1) | 0.56       | 2.5447     |
|           |         |     |     |     |       |        | Be-Nb(2) | 0.34       | 2.5888     |
|           |         |     |     |     |       |        | Be-Nb(3) | 0.10       | 2.6360     |
|           |         |     |     |     |       |        | Nb-Nb    | 0.33       | 2.9283     |

**Table 5:** The computed density $\rho$ (in gm/cm$^3$), transverse ($V_t$), longitudinal ($V_l$), and average sound velocity $V_m$ (m/s) and Debye temperature $\Theta_D$ (K) of Nb$_3$Be and Nb$_3$Be$_2$ phases.

| Compounds | $\rho$  | $V_t$  | $V_l$  | $V_m$  | $\Theta_D$ |
|-----------|---------|--------|--------|--------|-------------|
| Nb$_3$Be  | 7.33    | 2793.23| 5576.25| 3133.15| 368.36      |
| Nb$_3$Be$_2$ | 6.87  | 3295.04| 6086.74| 3677.12| 450.91      |
| Nb$_3$Ga  | 8.33$^a$| 2376$^a$| 5219$^a$| 2678$^a$| 308.0$^a$, 280.71$^b$ |

$^a$Ref. 45; $^b$Ref. 46