Numerical Investigation of the Stability and Spintronic Properties of Selected Quaternary Alloys

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ABSTRACT

The use of electronic charge and spins (spintronics) has been proposed for much better data storage. This class of material is believed to have excellent capability for data integrity, low dynamic power consumption and high-density storage that showcases excellent protection against data loss. The spintronic and related properties have been investigated on four newly proposed quaternary alloys (NbRhGeCo, NbRhGeCr, NbRhGeFe and NbRhGeNi) through the first-principles calculation method of the Density Functional Theory (DFT). Specifically, the phonon frequencies, elastic stabilities, and the electronic structure were systematically studied in the full Heusler structure. The results predict that NbRhGeFe and NbRhGeCr are elastically and structurally stable. Both NbRhGeFe and NbRhGeCo are half-metals with ferromagnetic character, but NbRhGeCo is unfortunately elastically unstable. NbRhGeCr and NbRhGeNi are non-magnetic metallic alloys in their spin channels. All the results predict NbRhGeFe to be the only suitable among all the four alloys for spintronic application.

Keywords: Exchange-splitting, Ferromagnetism, Polarization ratio, Spintronic.

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I. INTRODUCTION

The world has witnessed digital revolution (robotics, artificial intelligence, machine learning etc.). This has led to innovations, such as the robotic waiters, driver-less taxis, e-commerce, and tele-conferencing/medicine, which will continue to increase productivity. In all of these, data acquisition, storage, and transmission – both in size and integrity are cardinal to achieving the various objectives of modern-day technology. The traditional Non-Volatile Memories (NVMs) such as the Compact Disk, which can be Read or Written into (CD-R/W) and Hard Disk Drives (HDDs) uses magnetic material and retain their content even when their electric power is switched off. The NVMs are very sensitive to external magnetic fields and thermal fluctuations [1], [2] in which their data are easily lost when intentionally or accidentally exposed. It is also difficult to achieve higher storage density and capabilities with traditional NVMs, because applications using them do suffer from high static power caused by intrinsic current leakage and dynamic power consumption due to long interconnection delays [3]. The search for a better storage media led to the use of spin and charge (spintronics) for data storage. The technology for spintronic applications has created many nano devices, including spin valves and the Magnetic Tunnel Junction (MTJ) valve which has increased the memory capacity of HDDs more than 1000 times in the last ten years [4], [5]. In terms of speed, non-volatility and high data density, spintronic devices are very attractive. The Spin Transfer Torque Magnetic Random Access Memory (STT-MRAM) as an example can allow power-off in the standby state [6]. Spintronic memory devices are able to reduce dynamic power

loss while providing nearly infinite endurance which is required in high density and repeated-access memory medium.

The spintronic phenomenon was first described around 1988 through the Giant Magneto-resistance effect (GMR). The spin valve, which is the active element in the read head of HDD storage device use the GMR effect. Following the discovery of GMR, other technologies that utilizes the spintronic effect includes the Tunnel Magneto Resistance (TMR) and the Magnetic Tunnel Junction (MTJ), which has been in use for developing Magnetic Random Access Memory (MRAM) devices. The category of materials already proposed for spintronic applications are majorly magnetic materials [7]-[11], topological insulators [12], [13] and magnetic semiconductors [14]-[20]. The development of the spin Field Effect Transistor had showed that spintronic devices can only be realized with ferromagnetic semiconductors or metals [21]. For the sake of high Curie temperature and diverse magnetic phenomenon, materials with the Heusler structure have been shown to be very effective for formulating spintronic devices [22]-[24].

In a recent study, NbRhGe was predicted to be elastically and structurally stable with an indirect energy bandgap [25]. Given its optimum mechanical properties, it is the intention of the present study to predict new properties – particularly those relevant to data storage using NbRhGe as the base material. Therefore, magnetic elements are added into NbRhGe using the full Heusler structure. The selected elements are nickel (Ni), chromium (Cr), cobalt (Co) and iron (Fe). They are transition metals belonging in the d-block of the periodic table. Their electronic structure are: Ni =

($3d^8 4s^2$), Cr = ($3d^5 4s^1$), Fe = ($3d^6 4s^2$) and Co = ($3d^7 4s^2$) respectively. Among other things, the elastic as well as the dynamic stability of each composition are investigated. The overview of the methodology used in the computation is given in section 2. The results of the calculation alongside relevant discussion are given in section 3. The work done is finally summarized in section 4.

II. COMPUTATIONAL DETAILS

The crystal structure used for simulating NbRhGeX (X= Cr, Co, Fe, Ni) is shown in Fig.1. It is a face centred cubic structure (space group = F43m). Its Wyckoff atomic coordinates are 4a (0, 0, 0) 4b ($\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$), 4c($\frac{1}{4}$, $\frac{1}{4}$, $\frac{1}{4}$) and 4d($\frac{3}{4}$, $\frac{3}{4}$, $\frac{3}{4}$). The structure can take maximum of four elements, where the elements can come from same group or different element groups. All the calculations were performed with the Quantum Espresso ab initio code [26]. The generalized gradient approximations [28], was used to treat the electron exchange correlation potential within the Kohn-Sham equation of DFT [27]. Acceptable results were obtained when integration over the Brillouin-zone was done using shifted k-points of 1000 ($10 \times 10 \times 10$) according to the Monkhorst-Pack scheme [29]. The criterion for energy convergence was 10^{-4} Ry. The first task carried out was geometry optimization, where the potential energy surface was sampled repeatedly until minima forces on the atoms were obtained. Each alloy was optimized for the non-magnetic, ferromagnetic and antiferromagnetic states. After obtaining the ground state structure, the formation (E^F) and cohesive (E^C) energies were evaluated using (1) and (2).

$$E^F = E_t^{Xb} - E_t^{Ab} - E_t^{Bb} - E_t^{Cb} - E_t^{Db} \quad (1)$$

$$E^C = E_t^{Xb} - E_t^{A^{at}} - E_t^{B^{at}} - E_t^{C^{at}} - E_t^{D^{at}} \quad (2)$$

where E_t^{Xb} is the bulk ground state energy for NbRhGeX (X= Cr, Co, Fe, Ni) while E_t^{Ab} through E_t^{Db} and $E_t^{A^{at}}$ through $E_t^{D^{at}}$ are the ground state energy for the participating elements (Nb, Rh, Ge, Fe/Cr/Co/Ni) in their bulk states and the energies of each isolated atoms in their respective structures.

Fig. 1. Illustration of the full-Heusler (L2₁) structure. The site preference for Nb, Rh, Ge and Co/Ni/Cr/Fe are given in the legend.

The ground state lattice constant and bulk modulus were calculated using the Murnaghan's equation of state [30]. Being cubic, there are three elastic constants (C_{11} , C_{12} , C_{44})

that fully describes the mechanical properties of NbRhGeX (X= Cr, Co, Fe, Ni). The procedures followed to obtain these elastic constants are as follows [31]. A strain was applied to the crystal and the energy versus the strain was measured, with the elastic constant determined from the curvature of this function at zero strain. Two types of lattice strain were applied - a volume-conserving orthorhombic strain:

$$\varepsilon = \begin{pmatrix} x & 0 & 0 \\ 0 & -x & 0 \\ 0 & 0 & x^2/(1-x^2) \end{pmatrix}, \quad (3)$$

whose total energy is an even function of distortion x :

$$\Delta E(x) = \Delta E(-x) = V(C_{11} - C_{12})x^2 + \theta[x^4] \quad (4)$$

and a monoclinic volume-conserving strain:

$$\varepsilon = \begin{pmatrix} 0 & \frac{x}{2} & 0 \\ x/2 & 0 & 0 \\ 0 & 0 & x^2/(4-x^2) \end{pmatrix} \quad (5)$$

whose total energy dependence is of the form:

$$\Delta E(x) = \Delta E(-x) = \frac{1}{2}VC_{44}x^2 + \theta[x^4] \quad (6)$$

The value of the distortion x , was varied from zero (for the equilibrium state) to $\pm 5\%$. The elastic constant values are obtained from the derivatives of ΔE with respect to x^2 . After obtaining the single-crystal elastic constants, the related properties such as the bulk modulus can be evaluated. The Hill average for polycrystal moduli [32] is considered better in terms of accuracy and the expression for the bulk modulus for a cubic crystal is:

$$B = C_{11} + 2C_{12}/3 \quad (7)$$

Other properties that can be evaluated from the elastic constants includes the shear (G) and Young's modulus (E), Frantsevich's ratio (G/B), Zener anisotropy factor (A) [33], Kleinman internal-displacement parameter (ζ) [34], Poisson's ratio (ν), sound velocity (v_m) and the Debye temperature (Θ_D) [35] as well as the Vicker's hardness index (H_v) [36]. The expressions for these elastic constant dependent properties are given in (8) through (16).

$$G_R = 5(C_{11} - C_{12})C_{44}/[4C_{44} + 3(C_{11} - C_{12})];$$

$$G_V = C_{11} - C_{12} + 3C_{44}/5 \quad (8)$$

where

$$G = G_R + G_V/2 \quad (9)$$

$$E = 9BG/3B + G \quad (10)$$

$$\nu = 3B - 2G/2(3B + G) \quad (11)$$

$$C' = C_{12} - C_{44} \quad (12)$$

$$A = 2C_{44}/C_{11} - C_{12} \quad (13)$$

$$\zeta = C_{11} + 8C_{12}/7C_{11} + 2C_{12}, \quad (14)$$

$$H_V = 2(G^3/B)^{0.585} - 3, \quad (15)$$

$$v_l = \sqrt{1/3\rho[3B+4G]}; \quad v_t = \sqrt{G/\rho}; \quad v_m = [1/3(2/v_t^3 + 1/v_l^3)]^{-1/3};$$

$$\Theta_D = \hbar/k_B [3n/4\pi(N_A\rho/M)]^{1/3}v_m \quad (16)$$

where the Debye temperature (Θ_D) is a function of the Boltzmann constant (k_B), the Plank constant ($\hbar$), the number of atoms per formula unit (n), the Avogadro constant (N_A), ρ is the density of the material and M is the molecular weight.

The phonon frequencies were calculated as a second-order derivative of the total energy with respect to atomic displacements using the Density Functional Perturbation Theory (DFPT) [37].

III. RESULTS AND DISCUSSION

A. Ground-State Structure, Lattice Constants, Formation/Cohesive Energies and Elastic Constants

The ground state structures of NbRhGeFe and NbRhGeCo had lowest energy for the ferromagnetic state while NbRhGeNi and NbRhGeCr had their lowest energy for the non-magnetic state. At the zero-energy level (ground state), Nb preferred the 4a (0, 0, 0) position, while Ge occupied the 4b ($\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$) position. The Rh element locates in the 4c ($\frac{1}{4}$, $\frac{1}{4}$, $\frac{1}{4}$) position, with the 4d site ($\frac{3}{4}$, $\frac{3}{4}$, $\frac{3}{4}$) occupied by Fe/Cr/Co/Ni respectively. The lattice constants (L^C), formation/cohesive (E^F/E^C) energies and the elastic constants as well as the related mechanical properties are given in Table I. A negative value for E^F is an indication of a thermodynamically feasible composition. The cohesive energies are negative and large enough, predicting strong bonding forces in the compounds. Any material for

engineering purpose must have mechanical stability. From the elastic constants, the stability criteria for cubic lattices according to Born [38] are: $C_{11}-C_{12} > 0$, $C_{11} > 0$, $C_{44} > 0$ and $(C_{11}+2C_{12}) > 0$. The results in Table 1 predict that NbRhGeFe and NbRhGeCr are mechanically stable while NbRhGeCo and NbRhGeNi are not stable.

The ductility or brittleness of a material plays key role in its application. Brittle material is not malleable while ductile materials are malleable and can accommodation a lot of deformation before it is fractured. The Pugh and Frantsevich ratios provide easy ways to theoretically evaluate brittleness or ductility in a material. When the Pugh ratio (B/G) is ≥ 1.75 such material is ductile, else it is brittle [39]. On the other hand, a material is considered to be ductile if its Frantsevich's ratio (G/B) is ≤ 1.06 , else it is brittle [40]. Therefore, the results in Table 1 predicts that NbRhGeFe and NbRhGeCr are ductile alloys ($B/G > 1.75$ and $G/B < 1.06$) at ambient conditions while NbRhGeNi and NbRhGeCo are not mechanically stable. The Cauchy pressure (C_p) is another reliable way of checking for ductility or brittleness in a material [41]. A negative value for C_p would indicate a brittle material, else it is ductile. The C_p result further predicts that NbRhGeFe and NbRhGeCr should be ductile in alloys. The Kleinman parameter (ζ) is basically used to determine the ease of bond bending to bond stretching. With $\zeta = 0$, bond stretching is more favored is the material than bending while bond bending occurs more than stretching when $\zeta = 1$ [42]. The ζ results, predicts higher percentage of bonding stretching in the alloys. This further confirmed that NbRhGeFe and NbRhGeCr should be ductile alloys.

The hardness test for NbRhGeX ($X = \text{Fe, Co, Ni, Cr}$) was theoretically done using the Vicker's hardness (H_V) calculation method. A material is considered hard if its Vicker hardness is ≥ 40 GPa [43]. According to the results in Table I, NbRhGeFe and NbRhGeCr are predicted to be extremely hard materials while H_V for NbRhGeNi and NbRhGeCo cannot be determined due to their mechanical instability.

TABLE I: CALCULATED ISOTROPIC BULK MODULUS B, SHEAR MODULUS G, YOUNG'S MODULUS E, FRANTSEVICH'S RATIO (G/B), ELASTIC CONSTANTS (C_{11} , C_{12} , C_{44}), ZENER ANISOTROPY FACTOR A, KLEINMAN PARAMETER Z, POISSON'S RATIO N, VICKER'S HARDNESS INDEX H_V , SOUND VELOCITIES (V^T , V_L , V_M), AND THE DEBYE TEMPERATURE Θ_D , FOR NBRHGE X ($X = \text{Cr, Co, Fe, Ni}$) ALLOYS

Calculated	NbRhGeCr	NbRhGeFe	NbRhGeNi	NbRhGeCo
L^C (Å)	6.140	6.129	6.139	6.136
E^c (eV)	-364.012	-457.192	-441.613	-440.102
E^F (eV)	-0.798	-1.426	-1.374	-1.448
B (GPa)	203.513	198.939	195.1222	194.5660
B_0 (GPa)	203.820	201.550	202.579	196.782
G (GPa)	58.609	16.282	-67.626	-0.263
Frantsevich's ratio (G/B)	0.289	0.081	-0.345	-0.00135
Pugh (B/G)	3.465	46.463	-2.895	-741.741
E (GPa)	160.467	47.537	-228.847	-21.427
C_{11} (GPa)	273.959	199.395	120.579	128.752
C_{12} (GPa)	168.745	198.597	232.394	2281.090
C_{44} (GPa)	62.988	52.350	-66.301	7.802
A	0.004	0.939	1.185	-0.007
ζ	0.720	0.997	1.512	3.363
ν	0.369	0.427	0.677	0.569
H_V (GPa)	84.283	177.698	-----	-----
v_t (m/s)	2497.566	1329.691	-----	-----
v_l (m/s)	5478.104	4894.657	3464.292	11701.070
v_m (m/s)	2792.945	1505.992	-----	-----
Θ_D (K)	347.562	182.069	-----	24.650
C_p (GPa)	105.757	146.247	298.694	2273.288
μ_B	0.01	1.63	0.00	1.48

Materials that are required to take complex shapes during engineering processes (such as data storage devices) need to have high bonding strength [44], [45]. The bulk modulus (B), which measures the resistance of a material to external deformation, together with the materials resistance to shape change via shearing forces (i.e., the shear modulus, G) and the degree of stiffness of the material (i.e., the Young's modulus Y) can together be used to understand the bonding strength of a material [46]-[49]. When the results for B , G , Y are taken together with the already discussed H_v , C_p or G/B then one can conclude that NbRhGeFe and NbRhGeCr are strong alloys with expected high yield stress. Incidentally, the equation of states derived bulk modulus (B_0) and the one obtained from the elastic constants (B) are only apart by about 1.31% for NbRhGeFe and merely 0.15% for NbRhGeCr. This is a testimony to the high degree of self-consistency of the present calculation.

The relationship between the transverse and longitudinal strains along the elastic loading direction is called the Poisson's ratio (ν). The type of bond existing in a material can be gauged, using the Poisson ratio. If $\nu \approx 0.1$, covalent bonding is predicted, if $\nu \approx 0.23$ it is ionic and the bonding is metallic if $\nu \approx 0.33$ [50], [51]. The ν results in Table I, predicts that NbRhGeFe and NbRhGeCr should exhibit metallic bond.

B. Electronic Structure and Magnetic Properties

The calculated total magnetization (μ_B) for NbRhGeFe, NbRhGeCr, NbRhGeCo and NbRhGeNi are given in Table 1. NbRhGeFe ($\mu_B = 1.6$) and NbRhGeCo ($\mu_B = 1.4$) can be predicted to be magnetic due to their positive magnetic moments. The Density of States (DoS) result is given in Fig.

2 (a) to (d). A very strong exchange splitting can be seen (characteristic of a ferromagnet) at the Fermi level (E_F) between the up-spin channel and the down-spin channel of NbRhGeFe and NbRhGeCo. Because NbRhGeCr and NbRhGeNi are non-magnetic, their DoS lacked exchange-splitting along the spin channels at E_F . Magnetic half-metals are required for spintronic applications. The band structure along the high symmetry points for the up-spin and down-spin channels are shown in Figs. 3 & 4. All the four alloys showed zero energy band gap (characteristic of metals) in their up-spin channels (see Figs. 3(b), 3(d), 4(b) and 4(d)), while only NbRhGeFe and NbRhGeCo showed indirect energy band gap (characteristic of a semiconductor) for the down-spin channels (see Figs. 3 (a) & (c)). The GGA predicted band gap for NbRhGeFe was 0.301 eV and 0.644 eV for NbRhGeCo.

C. Phonon Dispersion

The phonon dispersion provides a valid tool to evaluate structural stability for a system. The calculated phonon curve along high symmetry directions in the Brillouin zone for NbRhGeX ($X = \text{Fe, Co, Ni, Cr}$) are shown in Fig. 5 (a) through (d). A structurally stable structure is obtained when the frequency of all phonons across Brillouin zone are positive at absolute zero temperature. Otherwise, the structure is unstable [52]. It can be observed that no imaginary vibration frequency appeared for NbRhGeCo, NbRhGeFe and NbRhGeCr while there was for NbRhGeNi. This suggests that NbRhGeFe, NbRhGeCo and NbRhGeCr are dynamically stable at absolute temperature.

Fig. 2. Calculated Density of states plot for NbRhGeX ($X = \text{Fe, Cr, Co, Ni}$).

Fig. 3. Calculated band-structure for NbRhGeX (X= Fe, Co) in the up-spin and down-spin channels.

Fig. 4. Calculated band-structure for NbRhGeX (X= Cr, Ni) in the up-spin and down-spin channels.

Fig. 5. Phonon dispersion curves for NbRhGeX (X = Fe, Cr, Co, Ni) alloys.

IV. CONCLUSION

Any data storage media that utilizes the spintronic application is expected to be a magnetic component with 100% polarization. Four quaternary alloys have been investigated for possible use in spintronics. The electronic, magnetic, mechanical, and structural properties of NbRhGeFe, NbRhGeCo, NbRhGeNi and NbRhGeCr have been evaluated. The electronic structure showed that only NbRhGeFe and NbRhGeCo are magnetic with the required 100% polarization. The other allied properties such as structure and mechanical stability was satisfied by NbRhGeFe while NbRhGeCo is unfortunately structurally and mechanically unstable. Conclusively and as summarized

in Table II, NbRhGeFe is predicted suitable for spintronic application while NbRhGeCr can be considered for use in other application areas but certainly not for spintronics. NbRhGeCo and NbRhGeNi are unstable compositions which does not deserve further attention. NbRhGeCr and NbRhGeFe are suggested for further studies especially at elevated temperature and pressure.

TABLE II: CRITERIA FOR SPINTRONIC APPLICATION AND HOW THE ALLOYS MEET THE REQUIREMENTS

Compound	100% Polarization	Mechanical Stability	Structure Stability	Magnetic Moment
NbRhGeCr	✗	✓	✓	✗
NbRhGeCo	✓	✗	✗	✓
NbRhGeFe	✓	✓	✓	✓
NbRhGeNi	✗	✗	✗	✗

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