

# The effect of systematic substitution of Nb with Ti on a potential high-temperature shape memory alloy: B2 NbRu

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**Abstract.** NbRu has been considered as a potential high-temperature shape memory alloy due to its high martensitic transformation temperature, however, it has poor superelasticity and other shape memory properties, which limits its applications. In this paper, the effect of systematic substitution of Nb with Ti on the structural, thermodynamic, and elastic properties of supercell  $2 \times 2 \times 2$  B2  $\text{Ru}_{50}\text{Nb}_{50-x}\text{Ti}_x$  spanning the entire composition range ( $x = 0, 6.25, 12.50, 18.75, 25.00, 31.25, 37.50, 43.75, 50$  at. %) is investigated using *ab initio* calculations. Elasticity results showed that the mechanical stability of the B2 phase improved with increasing Ti content, which could be associated with a decrease in transformation temperature. However, a suitable composition range within which  $C' \sim 0$ , resembling that of well-known TiNi, is identified. This predicts Ti addition to be effective in improving shape memory properties of B2 NbRu alloy.

## 1 Introduction

Nitinol (TiNi) is the most widely used shape memory alloy (SMA) for many applications due to its excellent shape memory properties such as high recovery strain of  $\sim 6\%$  and its superior superelasticity. However, due to its low martensitic transformation temperature ( $M_s$ ) of approximately 373K, its use is limited to applications with operational temperatures below 373K [1]. To overcome TiNi operation temperature limitation, SMAs that can operate at higher temperatures have been studied [2]–[4], including NbRu [3].

NbRu has an ordered cubic B2 phase structure at high temperature which undergoes a slight tetragonal distortion during cooling to form a tetragonal  $L1_0$  phase at  $\sim 1373\text{K}$ . Further cooling results in the additional formation of a monoclinic  $B19'$  phase at  $\sim 1158\text{K}$  [3]. Fonda et al. [3] indicated that the shape memory effect (SME) observed in NbRu is due to  $B2 \rightarrow L1_0$  phase transition, hence considered a potential high-temperature shape memory alloy (HTSMA). The recovery ratio has been found to increase with decreasing Nb content in B2  $\text{Nb}_{(50-x)}\text{Ru}_{(50+x)}$ , with a maximum recovery ratio of 88.9% for  $\text{Nb}_{47}\text{Ru}_{53}$  [5], whilst a recovery ratio of 50% has been reported for  $\text{Nb}_{50}\text{Ru}_{50}$  [3], [6].

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Furthermore, equiatomic NbRu has been reported to have a recovery strain of 4% after reheating the deformed sample at 1073K. Nonetheless, it was reported that cracking was observed on the tension surface indicating low critical stress for slip, hence cracking before reverse transformation could occur [3]. Low recoverable strain in NbRu has triggered several studies on this alloy, where researchers have added other alloying elements in a quest to improve its shape memory properties using both experimental and computational methods. Chang-Long et al. [7] studied the elastic properties of  $\text{Nb}_{(50-x)}\text{Ru}_{(50+x)}$  using the first-principles method. The results from their calculated elastic constants indicated that the tetragonal shear modulus ( $C'$ ) is negative at  $T = 0$  K, which is usually associated with the mechanical instability of the B2 phase [2], [8]. It was also noted that the increase in Nb increased the stability of the B2 phase, indicating a decrease in the  $\text{B2} \rightarrow \text{L1}_0$  martensitic transformation temperature ( $M_s$ ). In addition, Chang-Long et al. [9] later studied the effect of substituting Nb with Fe on the martensitic transformation of  $\text{B2 Ru}_{50}\text{Nb}_{50-x}\text{Fe}_x$ , as well as substituting Ru with Fe in  $\text{B2 Nb}_{50}\text{Ru}_{50-x}\text{Fe}_x$ , as Fe had been observed to increase the toughness of SMAs in previous studies. The heats of formation (HOF) results indicated that the thermodynamic stability of the B2 phase increased with increasing Fe content in  $\text{Nb}_{50}\text{Ru}_{50-x}\text{Fe}_x$ , and decreased with increasing Fe in  $\text{Ru}_{50}\text{Nb}_{50-x}\text{Fe}_x$ , indicating the B2 stabilizing effect of Nb [9], although here the effect of Fe addition on shape memory properties was not reported.

Moreover, the effect of Al addition in NbRu has been investigated by Benachird et al. [10]. From the calculated HOF, it was observed that  $\text{B2 Nb}_{50}\text{Ru}_{50}$  was the least thermodynamically stable with  $-0.137$  eV/atom, followed by the  $\text{Nb}_{34.55}\text{Ru}_{16.03}\text{Al}_{48.98}$  with  $-0.6125$  eV/atom and finally,  $\text{Nb}_{22.93}\text{Ru}_{52.42}\text{Al}_{24.59}$  with  $-0.6664$  eV/atom. These results were contradictory to those of Chang-Long et al. [7], [9], who reported that the reduction of Nb reduced the stability of the B2 phase. This further showed the effect of alloying elements on the phase stability or  $M_s$  of B2 NbRu as the stability seems to have improved with Al addition.

Collectively, it is evident that previous authors mostly reported the effect of alloying elements on the martensitic transformation temperature, of which from the computational studies [7], the data derived from elastic constants and shear modulus ( $C'$ ) were used to predict martensitic transformation behaviour of NbRu in comparison to that of TiNi [11]. To this point, the published work does not address the use of computational studies, elastic constants, in particular, to predict how additional alloying elements affect other shape memory properties of NbRu. This can be because most research is focused on  $M_s$ , which is an important feature of the use of NbRu as a HTSMA. However, it should be noted that for this alloy to be considered a successful HTSMA, other shape memory properties such as superelasticity and other mechanical properties must be improved.

Superelasticity is observed when a material is deformed above the high-temperature austenitic phase ( $A_s$ ). The formed martensite during the application of stress is referred to as stress-induced martensite (SIM). SMAs such as TiNi [11], CuZn [12], and AlCuTi [13] have shown excellent superelasticity. It has been previously reported that the stress required to produce SIM in these alloys increases with increasing temperature as it has a lower  $M_s$ , meaning that the required stress drops to zero at  $M_s$ . The formation of SIM is easily attainable in these alloys because of the underlying transformation mechanism associated with shape memory properties. For example, with TiNi, the transformation involves  $\text{B2} \rightarrow \text{B19}'$  [11], [12], [14]–[16] and for NbRu, it is  $\text{B2} \rightarrow \text{L1}_0$  [17]. With TiNi and CuZn, a few plates of SIM are formed with a habit plane that is sympathetic to the applied stress axis, i.e. shape deformation of a particular variant produces a maximum elongation of the specimen along the tensile axis, which is fully recovered upon release of stress. Whereas, the phase

transformation mechanism for the NbRu is rather complicated [17], thus resulting in poor mechanical and superelastic properties.

Therefore, using computational methods, it is possible to predict the composition within which the Ms is not decreased to below that of TiNi (maintaining SME in NbRu), whilst improving other shape memory properties of the NbRu alloy. It has been established that the small recovery ratios were observed with increasing Nb content in Nb<sub>(50+x)</sub>Ru<sub>(50-x)</sub>, therefore adjusting the Nb composition is a promising route towards improving superelasticity [9]. Additionally, Ti is known to be lighter with good corrosion resistance, hence considered more suitable for structural applications at elevated temperatures.

Thus, in this paper, the effect of systematically substituting Nb with Ti is reported, to predict the composition range within which shape memory properties of NbRu could be potentially improved.

## 2 Computational methodology

The B2 crystal structure was used to carry out all calculations reported in this study. The resulting geometry-optimized crystal structure was used to carry out all the calculations including structural, thermodynamic, and elastic properties of all considered compositions. Only valence electrons were considered through the use of ultrasoft pseudopotentials [18], [19]. All calculations were performed with pseudopotentials in generalized gradient approximation (GGA) [20] refined by Perdew, Burke, and Ernzerhof (PBE) [21].

The calculations were performed on a unit cell and 2x2x2 supercell of the B2 crystal structure with space group Pm3m consisting of 2 and 16 atoms, respectively, using density functional theory (DFT) based CASTEP code embedded in Materials Studio software package [19]. A plane wave energy cutoff of 700 eV and a k-point set of 16x16x16 and 8x8x8 for supercell and unit cell, respectively, were sufficient to converge the total energy of the considered systems. The effect of substituting Nb atoms with Ti on the structure, phase stability, and elastic properties was determined. The ternary compositions considered were of stoichiometry Ru<sub>50</sub>Nb<sub>50-x</sub>Ti<sub>x</sub>, spanning the entire composition range. All the ground-state structures were optimized using the Brayden-Fletcher-Goldfarb-Shanno (BFGS) minimization scheme. The convergence criterion of less than  $1 \times 10^{-5}$  eV/atom, the maximum residual forces of 0.03 eV/Å, maximum residual bulk stress of 0.05 GPa, and maximum atomic displacement of  $1 \times 10^{-3}$  Å were utilized.

## 3 Results and discussion

### 3.1 Structural and thermodynamic phase stability

Table 1 shows the theoretical lattice parameters and heats of formation ( $\Delta H_f$ ) for B2 Ru<sub>50</sub>Nb<sub>50-x</sub>Ti<sub>x</sub> as well as for TiNi. The calculated lattice parameters for the B2 crystal of NbRu are found to be in excellent agreement with both theoretical and experimental values reported in the literature. For comparison purposes, the lattice parameters for the ternary compositions were not found in the literature, but it was noted that the values decreased linearly with increasing Ti content. This can be attributed to the fact that the atomic radius of Nb is slightly larger than that of Ti [22] and also the thermal expansion of Ti is smaller than that of Nb [23], [24]. For testing the accuracy of deployed geometric parameters, the calculated lattice parameter of TiNi also showed good agreement with available theoretical and experimental data.

Also shown in Table 1 are the heats of formation for B2 Ru<sub>50</sub>Nb<sub>50-x</sub>Ti<sub>x</sub> and TiNi, calculated using Equation (1) [25]. Heats of formation is described as the enthalpy change

when one mole of a compound is formed from the constituent elements and is used to determine the thermodynamic stability of a given crystal structure.

$$\Delta H_f = E_{Total} - \sum_i x_i E_i \quad (1)$$

where  $E_{Total}$  is the total energy of the compound and  $E_i$  is the calculated total energies of the element  $i$  and  $x_i$  is the concentration of element  $i$  in the compound in their respective ground-state structures. A phase is considered thermodynamically more stable when the value of formation energy is more negative.

All the investigated B2 phases in the current study were found to be negative, indicating that they are all thermodynamically feasible at 0 K. It was observed that the B2 phase became more stable with increasing Ti content towards B2 TiRu, which is known for being highly stable [26], [27]. On the other hand, the thermodynamic stability of the B2 phase with the 18.75 at. % Ti composition is comparable to that of TiNi, meaning that the energy released during the formation of B2 phase will be similar for both alloys. In other words, the activation energy required to form B2 phase by the exothermic reaction in 18.75 at. % Ti composition is equal to that of TiNi. All the calculated heats of formation were found to be in accordance with experimental and theoretical data available in the literature, as presented in Table 1.

**Table 1.** Lattice parameters and heats of formation  $[-\Delta H_f]$  for investigated B2  $Ru_{50}Nb_{50-x}Ti_x$  and TiNi

Composition x (at. %)	Lattice parameters, (Å)		$-\Delta H_f$ (atom/eV)	
	Current study	Literature	Current study	Literature
0	3.170	3.170 [5],[28] 3.180*[29],[30]	0.168	0.163 [28] <sup>a</sup> 0.152 [28] <sup>b</sup> 0.137*[10]
6.25	3.159	-	0.246	-
12.50	3.150	-	0.309	-
18.75	3.138	-	0.390	-
25.00	3.127	-	0.464	-
31.25	3.115	-	0.540	-
37.50	3.104	-	0.611	-
43.75	3.092	-	0.682	-
50.00	3.080	3.060*[26]	0.744	0.770 [27] 0.80*[31]
TiNi	3.015	3.019 [32]	0.403	0.353 [34]

		3.013*[33]		0.351*[33]
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\*Experimental value

<sup>a</sup>US-PP (GGA) [28]

<sup>b</sup>PAW (GGA) [28]

### 3.2 Elastic properties and mechanical phase stability

The single-crystal elastic constants for B2 Ru<sub>50</sub>Nb<sub>50-x</sub>Ti<sub>x</sub> and TiNi lattice structures were calculated in the current study to determine the effects of systematically substituting Nb with Ti on the mechanical stability and elastic properties of the B2 phase, as presented in Fig. 1. For the cubic crystals, the minimum energy conformation requires about four simulations. The derivation of coefficients requires an additional three or four simulations per independent coefficient. Fifteen energy calculations are required from which three independent constants C<sub>11</sub>, C<sub>44</sub>, and C<sub>12</sub> are derived for a cubic crystal. The mechanical stability criteria for the cubic system are explained in [35] and are given as follows:

$$C_{11} - C_{12} > 0; C_{44} > 0; C_{11} + 2C_{12} > 0 \tag{2}$$

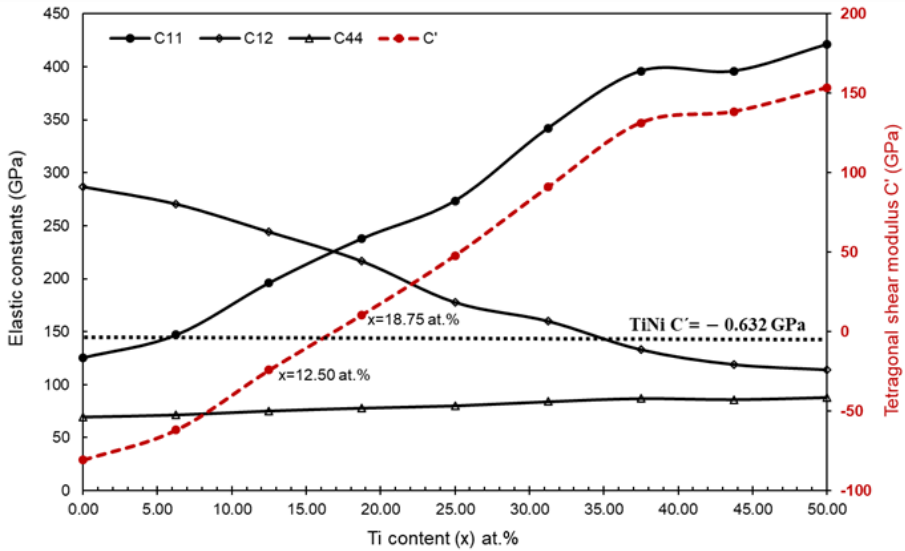
The tetragonal and trigonal deformations for the calculation of the C' and C<sub>44</sub> were applied to the cubic structure with equilibrium volume, where C' is expressed as:

$$C' = \frac{C_{11} - C_{12}}{2} \tag{3}$$

The C' corresponds to the {110}{110} tetragonal shear modulus, which is related to the formation of basal-plane-based martensites. On the other hand, the C<sub>44</sub> is the {001}{110} shear modulus, presenting a monoclinic distortions. Thus as such, a positive C' has been associated with an indication of the mechanical stability of a crystal. All the calculated elastic constants were positive, however, C' was found to be negative for compositions with less than 18.75 at. % Ti. This is to what other authors have reported that NbRu is unstable and undergoes a phase transformation at high temperatures, leading to instability of the B2 phase at 0 K. Upon increasing Ti content ≥ 18.75 at. %, the C' became positive.

On the other hand, it has been reported that the B19' phase of TiNi originates from the additional softening of C<sub>44</sub>, besides the softening of C' [36], which means that C' should be used in conjunction with C<sub>44</sub> to determine phase stability. However, here the results showed that C<sub>44</sub> is independent of Ti content, whereas C' increased with Ti content. This implies that stronger Ti-Ru bonds are formed, thus stabilizing the B2 phase during tetragonal deformations.

The C' for TiNi is closer to zero (-0.6 GPa), implying less stress is required to induce martensite. However, contrary to many studies, the negative C' here does not independently correspond to higher Ms, but simply depicts low resistance to tetragonal shear which is needed to form SIM. The Ms has been found to correspond to the softening of both C' and C<sub>44</sub> in TiNi [11]. Furthermore, the current study found the anisotropy factor (A= C<sub>44</sub>/C) to be -74, which can be associated with high flexibility in TiNi. Therefore, a composition range within which C' approaches zero, i.e. closer to that of TiNi has been identified for B2 Ru<sub>50</sub>Nb<sub>50-x</sub>Ti<sub>x</sub> between 12.50 and 18.75 at. % Ti. This composition range can then be tested experimentally to identify the actual Ms. The calculated anisotropy factor (A) for the "C'~0" composition range is between -3 and 7. Drawing from B2 TiNi elasticity data, it is evident that the stability of B2 is necessary for the promotion of superelasticity, thus within the identified composition range, the shape memory properties could be improved.



**Fig. 1.** The calculated elastic constants and tetragonal shear modulus  $C'$  of investigated B2  $Ru_{50}Nb_{50-x}Ti_x$  and TiNi

## 4 Conclusions

The effect of adding Ti into B2 NbRu has been investigated in the current study. The thermodynamic phase stability of the B2 phase increased with increasing Ti content at 0 K. The elastic constants revealed that the B2 phase becomes more mechanically stable with increasing Ti content. Furthermore, a composition range has been predicted, within which the mechanical and shape memory properties can be improved for structural applications. Moreover, the B2-stabilising effect of Ti indicated that  $Ru_{50}Nb_{50-x}Ti_x$  alloy compositions may also be considered for low-temperature applications such as biomaterials, taking advantage of its low magnetic susceptibility which is beneficial for diagnostic scans.

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