

Data-driven study of composition-dependent phase compatibility in NiTi shape memory alloys

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ABSTRACT

The martensitic transformation in NiTi-based Shape Memory Alloys (SMAs) provides a basis for shape memory effect and superelasticity, thereby enabling applications requiring solid-state actuation and large recoverable shape changes upon mechanical load cycling. In order to tailor the transformation to a particular application, the compositional dependence of properties in NiTi-based SMAs, such as martensitic transformation temperatures and hysteresis, has been exploited. However, the compositional design space is large and complex, and experimental studies are expensive. In this work, we develop an interpretable piecewise linear regression model that predicts the λ_2 parameter, a measure of compatibility between austenite and martensite phases, and an (indirect) factor that is well-correlated with martensitic transformation hysteresis, based on the chemical features derived from the alloy composition. The model is capable of predicting, for the first time, the type of martensitic transformation for a given alloy chemistry. The proposed model is validated by experimental data from the literature as well as in-house measurements. The results show that the model can effectively distinguish between $B19$ and $B19'$ regions for any given composition in NiTi-based SMAs and accurately estimate the λ_2 parameter.

1. Introduction

Nickel-Titanium (NiTi) based shape memory alloys (SMAs) [1–4] are distinguished for their capability to undergo reversible shape changes in response to external stimuli, making them invaluable for mechanical actuation and superelasticity across various industries. The shape memory effect in these alloys is attributed to reversible martensitic transformation from a high-temperature austenite phase, characterized by a $B2$ cubic crystal structure, to a low-temperature martensite phase, which can adopt either an orthorhombic $B19$ or a monoclinic $B19'$ or a rhombohedral R -phase structure [5–8]. The characteristics of these transformations directly influence their application potential. Notably, the transformation temperatures of NiTi SMAs are critical in defining their operational temperature range [3,4,9–12], while the associated thermal hysteresis plays a crucial role in energy conversion efficiency, energy absorption in mechanical dampers, and in accelerating the functional fatigue of mechanical switches [6,13].

The hysteresis and transformation temperature characteristics of NiTi-based SMAs are significantly influenced by their composition, leading to a vast and intricate compositional design space. Early research, such as the one by Wang (1965) [14], revealed the dependency of transformation temperatures on the Ni content within the NiTi stoichiometric range. Subsequent experimental efforts expanded this understanding by exploring the effects of alloying NiTi with elements like Al, Au, Co, Cu, Fe, Hf, Mn, Pd, Pt, and Zr in ternary, quaternary, quinary, and multi-component alloy systems [6,15–27]. However, traditional experimental approaches are costly and can only explore a limited portion of the alloy design space.

In recent years, the advent of sophisticated data-driven methods has allowed researchers to create models for predicting transformation temperatures. These models utilize compositional atomic percentages [28–30] and, in more advanced approaches, incorporate physical and chemical properties as features [31–38]. While these models show an acceptable level of prediction accuracy for transformation tempera-

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Table 1

Martensitic transformation characteristics from the in-house experimental data: The Latent Heat (L) is calculated as the average enthalpy change during the austenite-to-martensite and martensite-to-austenite phase transitions. SHT stands for solution heat treatment.

Composition (at%)	$M_s(^{\circ}\text{C})$	$M_f(^{\circ}\text{C})$	$A_s(^{\circ}\text{C})$	$A_f(^{\circ}\text{C})$	$\Delta T(^{\circ}\text{C})$	$\theta_c(^{\circ}\text{C})$	$L(\text{J}/\text{cm}^3)$	Processing
$\text{Ni}_{32.5}\text{Ti}_{36.5}\text{Hf}_{14.0}\text{Cu}_{17.0}$	13	3.4	25.5	37	23.1	19.7	99.1	SHT (950 $^{\circ}\text{C}$, 24 h)
$\text{Ni}_{32.5}\text{Ti}_{32.5}\text{Hf}_{18.0}\text{Cu}_{17.0}$	43	26.6	57.8	77	32.6	51.1	128.9	SHT (950 $^{\circ}\text{C}$, 24 h)
$\text{Ni}_{42.7}\text{Ti}_{25.3}\text{Hf}_{25.0}\text{Cu}_{7.0}$	299	247.4	332.1	344.5	65.1	305.8	252.9	SHT (1050 $^{\circ}\text{C}$, 24 h)
$\text{Ni}_{41.9}\text{Ti}_{23.1}\text{Hf}_{27.0}\text{Cu}_{8.0}$	191.5	132.1	195.7	221.7	46.9	185.3	160.1	SHT (950 $^{\circ}\text{C}$, 24 h)
$\text{Ni}_{43.1}\text{Ti}_{23.9}\text{Hf}_{26.0}\text{Cu}_{7.0}$	286.4	237.8	312.5	327.1	57.7	290.9	268.9	SHT (1050 $^{\circ}\text{C}$, 24 h)
$\text{Ni}_{34.6}\text{Ti}_{38.4}\text{Hf}_{12.0}\text{Cu}_{15.0}$	38.9	25.1	50.7	59.5	23.1	43.6	130.7	SHT (1050 $^{\circ}\text{C}$, 24 h)
$\text{Ni}_{35.4}\text{Ti}_{22.6}\text{Hf}_{27.0}\text{Cu}_{15.0}$	70.8	43.6	90.6	99.7	38	76.2	127.9	SHT (1050 $^{\circ}\text{C}$, 24 h)
$\text{Ni}_{41.0}\text{Ti}_{24.0}\text{Hf}_{26.0}\text{Cu}_{9.0}$	299.5	250.8	327.6	341.7	59.5	304.9	249.2	SHT (1100 $^{\circ}\text{C}$, 24 h)

tures, their ability to forecast thermal hysteresis accurately remains a challenging area, highlighting the need for continued research and model refinement.

Thermal hysteresis in SMAs is mainly caused by energy dissipation during the martensitic transformation. This loss is primarily due to defect generation and internal friction, leading to an increased range of heating and cooling [6,13]. According to a theory proposed by James et al. (2005) [39], Cui et al. (2006) [40], and Zhang et al. (2009) [41], the thermal hysteresis of the martensitic transformation is primarily controlled by the number of low-stress martensite-austenite interfaces. As an ideal case, an infinite number of perfect, stress-free, and untwinned interfaces between austenite and martensite, referred to as full-phase compatibility, can be realized when a parameter— λ_2 —associated with the degree of crystallographic compatibility between austenite and martensite is precisely equal to 1. Although this ideal condition is never exactly attained, experimental results from NiTiAu, NiTiPt, NiTiCu, NiTiPd, NiTiHf, NiTiZr, and NiTiCuPd alloy systems [13,20] substantiate the idea that λ_2 in proximity to 1 leads to a large but finite number of low-stress compatible interfaces, resulting in a substantial reduction in thermal hysteresis. The λ_2 parameter depends directly on the martensite-austenite crystal structures and lattice parameters, which are impacted by alloy composition, so the λ_2 parameter provides a link between alloy composition and thermal hysteresis amenable to data-driven machine learning methods.

The λ_2 could be considered as an ideal alloy design parameter for SMAs due to its direct correlation with phase compatibility between martensite and austenite and its correlation with thermal hysteresis. However, the practical application of λ_2 is challenging because its value, which depends on the crystal structures and lattice parameters of the coexisting austenite and martensite phases, can only be determined through experimental analysis of an alloy already synthesized. Consequently, the development of a predictive model for λ_2 , based on more readily ascertainable parameters like alloy composition, is highly desirable. Such a model would enable the prediction of phase compatibility and thermal hysteresis in SMAs before synthesis and experimental investigation, greatly facilitating the design and optimization of these materials and overcoming the current limitations of retrospective determination.

In this work, we develop and experimentally validate an interpretable piecewise linear regression model that identifies the chemical and physical property ranges leading to either B19 or B19' transformations and also predicts the λ_2 parameter based on the chemical features derived from the alloy composition. This can enable a better understanding and design of SMAs with desired transformation characteristics, using data-driven methodologies.

2. Methods

2.1. Data

A comprehensive dataset comprising 178 data points of NiTi SMAs was amassed from existing literature [2,13,20,39,41–96]. This dataset

encompassed detailed descriptions of compositions, transformation temperatures, hysteresis, latent heat (enthalpy of transformation), density, lattice parameters, and λ_2 parameters. However, not all data points within this collection contain every measurement. For example, while some sources may provide extensive details on hysteresis, they might omit transformation temperatures, and others might focus on λ_2 parameters but not include lattice parameters. The data gathered predominantly are from experimental work conducted by various research groups. In an effort to maintain high fidelity, data derived from Density Functional Theory (DFT) computations were deliberately excluded due to potential concerns over their precision and variability in simulation settings. Additionally, we have added eight new data points from rigorous experimental investigations in quaternary SMA systems. Including these contributions, the total number of data points analyzed in our study amounts to 186.

For the samples we contributed to the data set, Differential Scanning Calorimetry (DSC) was used to measure Martensite start (M_s), Martensite finish (M_f), Austenite start (A_s), and Austenite finish (A_f) temperatures, and Latent heat (L). Details of the measured transformation characteristics are provided in Table 1. In this table critical temperature (θ_c) is calculated by averaging the transformation temperatures [41,44]. To calculate hysteresis (ΔT), we primarily utilized the formula $\frac{A_s + A_f - M_s - M_f}{2}$ [44]—we note that certain sources define hysteresis as $A_f - M_s$ [13,40]. For the literature data, when actual transformation temperature values were unavailable, we used the reported hysteresis value from the respective source.

The lattice parameters for in-house experiments were measured using low-temperature and high-temperature X-ray diffraction (XRD) analysis, as detailed in Table 2. The XRD analysis was conducted using a Bruker D8 Discover instrument with Copper $K\alpha$ radiation, covering a 2θ range of 20–80 $^{\circ}$ at a scan speed of 2 $^{\circ}$ /min. For the high-temperature austenite phase, samples were heated above their A_f temperature using a high-temperature XRD stage with a platinum heating strip to ensure full transformation into austenite, and then cooled above the M_s temperature while maintaining their austenitic state for the measurements. For the martensite phase, samples were first cooled to room temperature and then gradually heated to temperatures below the A_s temperature to ensure they were fully in the martensitic state before conducting the XRD experiments.

To calculate λ_2 values from the lattice parameters, the lattice deformation matrix B was utilized [2]:

$$B = \begin{bmatrix} \frac{a}{a_0} & 0 & \frac{\sqrt{2}c \cos(\beta)}{2a_0} \\ 0 & \frac{\sqrt{2}b}{2a_0} & 0 \\ 0 & 0 & \frac{\sqrt{2}c \sin(\beta)}{2a_0} \end{bmatrix}, \quad (1)$$

wherein a_0 is the lattice parameter of austenite phase with B2 structure and a, b, c ($a < b < c$), and β are lattice parameters of martensite phase with B19/B19' structure. The λ_2 parameter is the middle eigenvalue of the non-rotational part of the B matrix. We calculated the eigenvalues using Singular Value Decomposition (SVD). This can be expressed

Table 2

The experimental lattice parameters and the derived compositional features. The calculation of features, avg_first_ion_en_divi_voro_coord, dev_mol_vol, and δ is discussed in Section 3.1.

Composition (at%)	a_0 (Å)	a (Å)	b (Å)	c (Å)	β (°)	λ_2	avg_first_ion_en_divi_voro_coord	dev_mol_vol	δ
$Ni_{32.5}Ti_{36.5}Hf_{14.0}Cu_{17.0}$	3.093	3.112	4.069	4.925	103	0.93	0.673	2.324	9.51
$Ni_{32.5}Ti_{32.5}Hf_{18.0}Cu_{17.0}$	3.124	3.112	4.094	4.926	103.5	0.927	0.665	2.434	9.86
$Ni_{42.7}Ti_{25.3}Hf_{25.0}Cu_{7.0}$	3.119	3.085	4.123	4.856	101.3	0.935	0.651	2.684	10.7
$Ni_{41.9}Ti_{23.1}Hf_{27.0}Cu_{8.0}$	3.143	3.11	4.141	4.89	100.5	0.932	0.647	2.738	10.83
$Ni_{43.1}Ti_{23.9}Hf_{26.0}Cu_{7.0}$	3.12	3.124	4.11	4.901	103.1	0.931	0.649	2.718	10.79
$Ni_{34.6}Ti_{38.4}Hf_{12.0}Cu_{15.0}$	3.085	3.078	4.103	4.896	102.8	0.94	0.676	2.28	9.38
$Ni_{35.4}Ti_{22.6}Hf_{27.0}Cu_{15.0}$	3.136	3.128	4.131	4.907	102.1	0.931	0.647	2.71	10.66
$Ni_{41.0}Ti_{24.0}Hf_{26.0}Cu_{9.0}$	3.119	3.13	4.103	4.899	102.9	0.93	0.649	2.706	10.73

as $B = U\Sigma V^T$, wherein U , Σ , and V^T are distinct matrices. U is an orthonormal matrix of dimensional 3×3 formed from the eigenvectors of BB^T . V^T represents the transpose of another 3×3 orthonormal matrix; its values are derived from the eigenvectors of B^TB . Σ refers to a diagonal matrix, containing three diagonal elements, equal to the square root of positive eigenvalues found in BB^T . Σ is represented as λ_1 , λ_2 , and λ_3 , with the elements sequentially increasing in value as $0 < \lambda_1 < \lambda_2 < \lambda_3$ [2,5,97–99]. The `linalg.svd` function from the NumPy python library [100] was utilized for SVD calculations.

2.2. Model

We aimed to derive a regression model to predict λ_2 values based on the extracted chemical and physical features derived from alloy composition. To start, we employed HEACalculator package [101] and the Jarvis [102,103], Oliynyk [104], mat2vec [105], and Magpie [106] databases within the CBFV package [107] to generate a comprehensive set of chemical and physical features, resulting 4937 features. This extensive feature set was systematically analyzed by plotting each feature against the target to identify potential linear relationships. Our objective was to explore potential correlations between these features and the λ_2 values using the gathered data, aiming to discern identifiable trends within the dataset.

For the purpose of enhancing interpretability, we have opted for a piecewise linear regression model over more complex machine learning methods to facilitate a clearer understanding of the underlying relationships within the data. Furthermore, the predictive accuracy of the linear regression model was deemed sufficient, obviating the need for more complex methodologies. Linear regression models, in their simplest form, can be expressed as $y = \beta_1^T \mathbf{x} + \beta_0$. Here, the independent variables are represented by the vector $\mathbf{x}$, also known as the feature vector, while the dependent variable is y , referred to as the target variable. The regression model coefficients are contained in β_1 , indicating how changes in the corresponding input variables in $\mathbf{x}$ affect y . Meanwhile, the y-intercept is represented by β_0 , predicting the value of y when $\mathbf{x}$ equals zero [108]. Overall, this framework provides a useful approach for understanding and predicting the linear relationship between selected variables.

3. Results and discussion

3.1. Reduced-order model for λ_2 parameter and B19/B19' transformation pathways

Analyzing the available data, and plotting the compositional features against λ_2 values as the target of study, we have observed a correlation between λ_2 and the parameters outlined in Hume-Rothery rules [109–112]. According to these rules, the formation of a solid solution in binary alloy systems largely depends on several key parameters such as atomic size and electronegativity. To further the study of multi-component alloys, additional guidelines have been introduced for phase formation, which include the δ parameter [112,113], as well as considerations of molar volume and melting point [114].

For an alloy consisting of N elements, the δ parameter can be calculated using [112,113]:

$$\delta = \sqrt{\sum_{i=1}^N c_i \left(1 - \frac{r_i}{\bar{r}}\right)^2} \quad [1], \quad (2)$$

$$\bar{r} = \sum_{i=1}^N c_i r_i \quad [\text{pm}], \quad (3)$$

where c_i represents the atomic percentage of the i -th element, and $\frac{r_i}{\bar{r}}$ denotes the ratio of the radius of the i -th element to the weighted average radius of the elements in the alloy.

The weighted deviation of molar volume (dev_mol_vol) is calculated using [115]:

$$\text{dev_mol_vol} = \sum_{i=1}^N f_i |V_{m,i} - \bar{V}_m| \quad \left[\frac{\text{cm}^3}{\text{mol}}\right], \quad (4)$$

$$\bar{V}_m = \sum_{i=1}^N f_i V_{m,i} \quad \left[\frac{\text{cm}^3}{\text{mol}}\right], \quad (5)$$

where f_i is the fractional composition of the i -th component, $V_{m,i}$ represents the molar volume of the i -th component (commonly measured at standard conditions of 298 K and 1 atm), and $\bar{V}_m$ is the weighted average of molar volume. Given the established correlation between V_m and V_{cell} [116,117], which is inherently related to the cubic order of the atomic radius r^3 , a critical observation can be made from the comparison of Fig. 1.a and Fig. 1.b. This comparison elucidates that both parameters, δ and dev_mol_vol, underscore the significant influence of atomic size mismatch on λ_2 . This result was anticipated, as differences in atomic sizes within solid solutions cause lattice distortion, creating defects and altering energy barriers, which affect thermal hysteresis.

While there is a notable correlation observed between the δ and dev_mol_vol parameters and λ_2 , the differentiation between the B19 and B19' regions remains less distinct than desired. Alloys undergoing B19 transformation are characterized by low transformation hysteresis, emphasizing the importance of a clear delineation between these regions. In our pursuit of a more effective compositional characteristic, we turned our attention to two promising candidates: the first ionization energy and the Voronoi coordination number.

The first ionization energy represents the energy necessary to detach the outermost electron from an atom. This energy requirement is influenced by the electrostatic attraction between the electron and nucleus, as well as their relative distance. Decreasing the nuclear charge lessens this force, and enlarging the atomic radius increases the separation, both actions simplifying the process of electron detachment and thus reducing the ionization energy. Given that electronegativity reflects an atom's tendency to attract and retain electrons within a bond, an atom with a strong affinity for electrons generally demands more energy to liberate one of its electrons, resulting in a higher ionization energy [118,119]. The Voronoi coordination number is closely tied to

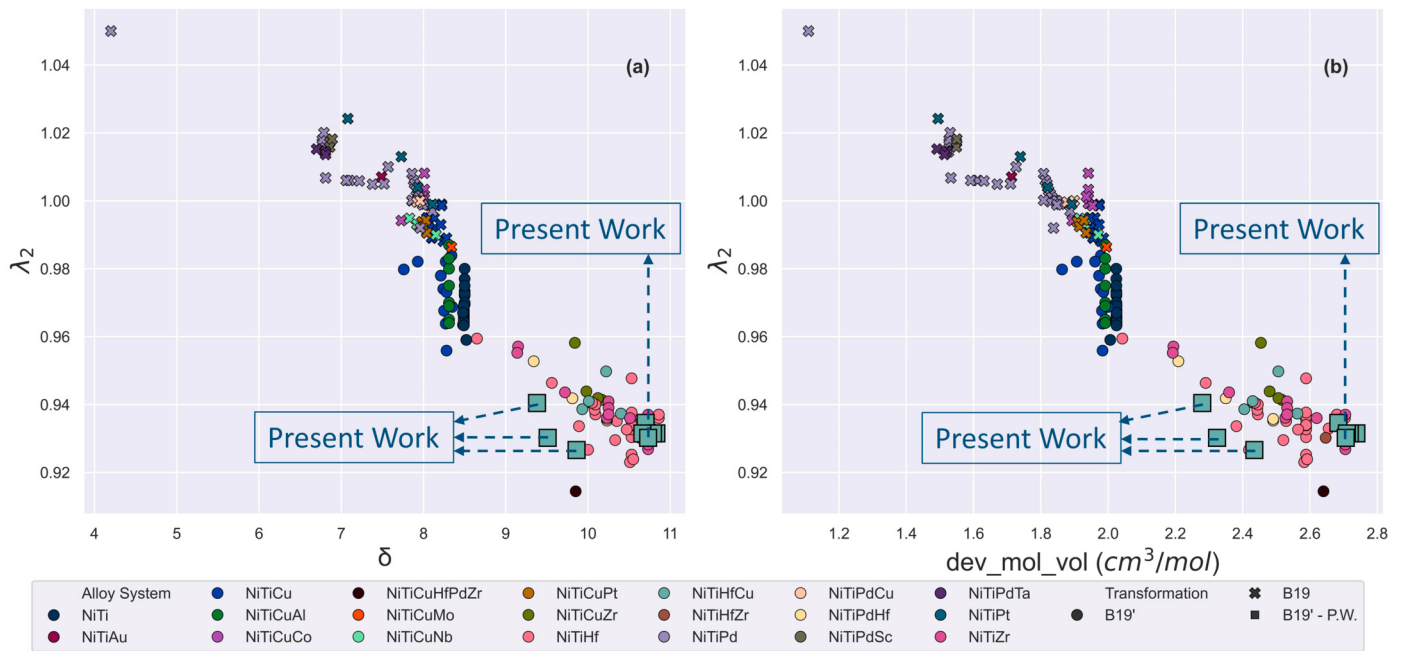


Fig. 1. Analysis of 178 literature-mined and 8 in-house experimental data points for λ_2 versus the generated features: (a) δ , and (b) dev_mol_vol . “Present Work” (P.W.) refers to data points generated in this work.

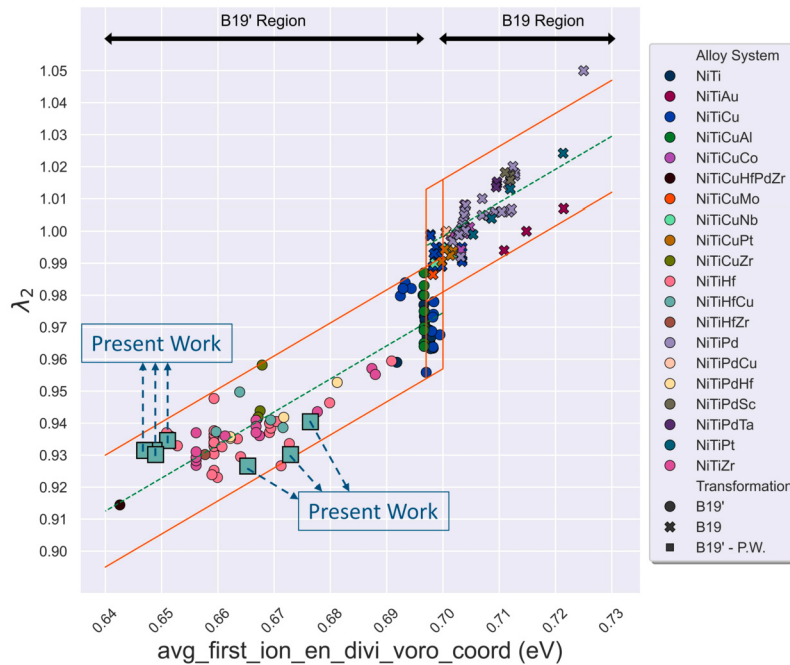


Fig. 2. Correlation analysis between λ_2 and $\text{avg_first_ion_en_divi_voro_coord}$: This graph highlights a notable correlation pattern between these two parameters. A clearly distinguishable transition zone is observed between the $B19$ and $B19'$ regions.

the number of nearest neighbors surrounding an atom in a given chemical environment. This number is a crucial determinant of the atomic radius, as it directly influences the spatial arrangement and packing efficiency of atoms within a structure [120,121].

We observed that the combination of these features, weighted average of quotient of the first ionization energy and the Voronoi coordination number (denoted as “ $\text{avg_first_ion_en_divi_voro_coord}$ ”), has a strong correlation with our target variable λ_2 . This super feature actually partitions the design space in half, and each half is extremely predictive of whether the transformation pathway is $B19$ or $B19'$. The

mentioned correlation is depicted in Fig. 2 and the super feature can be expressed as [115]:

$$\text{avg_first_ion_en_divi_voro_coord} = \sum_{i=1}^N f_i \cdot \frac{IE_{1,i}}{Vor_i} \quad [\text{eV}], \quad (6)$$

where $IE_{1,i}$ and Vor_i are the first ionization energy and Voronoi coordination number of i -th component, respectively. The summary of discussed features is provided in Table 3.

Our proposed model for predicting λ_2 values and type of transformation is based on this super feature ($x = \text{avg_first_ion_en_divi_voro_coord}$):

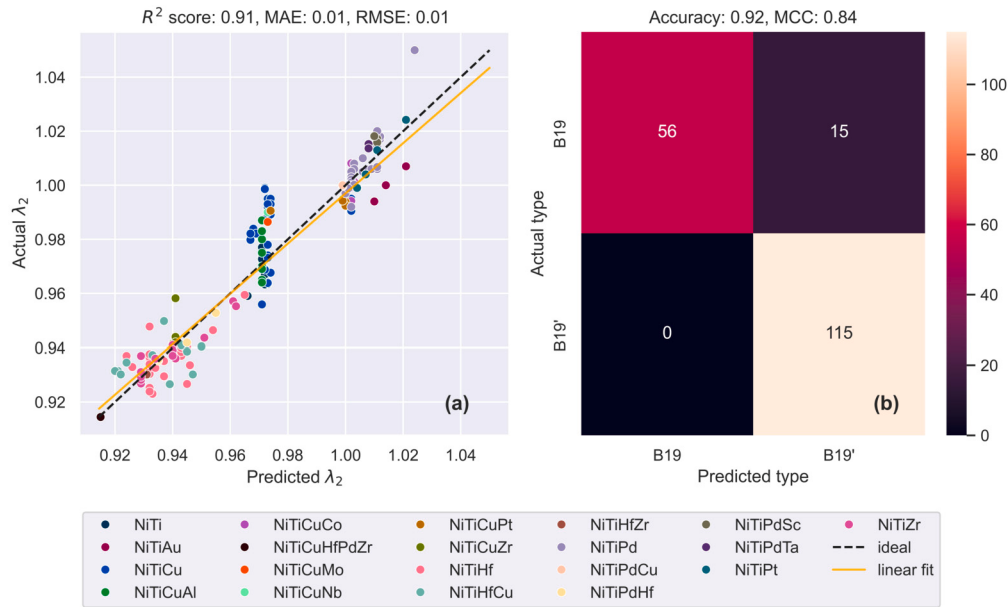


Fig. 3. The performance of the developed model for (a) λ_2 prediction, and (b) transformation type prediction.

Table 3

The summary of chemistry-dependent features to correlate with λ_2 values and crystal structure.

Symbol / Abbreviation	Equivalents
δ	Delta parameter
dev_mol_vol	Weighted deviation of molar volume
avg_first_ion_en_divi_voro_coord	Weighted average of the quotient of the first ionization energy and the Voronoi coordination number

$$\text{Model (x)} = \begin{cases} \lambda_2 = 1.0333x + 0.2512, \\ \text{type} = B19' & x < 0.700 \\ \lambda_2 = 1.0333x + 0.2752, \\ \text{type} = B19 & x \geq 0.700 \end{cases} \quad (7)$$

The model's performance was evaluated using the coefficient of determination (R^2), Mean Absolute Error (MAE), and Mean Square Error (RMSE) for λ_2 prediction [122,123]. The R^2 score was calculated as 0.91, MAE as 0.01, and RMSE as 0.1. For transformation type prediction, we employed accuracy and Matthews Correlation Coefficient (MCC) [124]. The accuracy and MCC were calculated as 0.92 and 0.84, respectively. The performance is outlined in Fig. 3. While accuracy measures the proportion of correct predictions out of all predictions made, the MCC is a balanced metric that considers true and false positives and negatives. The MCC is particularly useful when there is an imbalance in class sizes. All metrics were calculated using the `scikit-learn` [125] python library. These results show that combining atomic properties provides a valuable model with high accuracy to define not only the type of transformation, but also the range of λ_2 values for a given NiTi shape memory alloy, based solely on their composition.

It is crucial to recognize that the observed correlations between specific features and the λ_2 parameter in SMAs are statistical in nature and do not imply causation. The underlying causal mechanisms for these correlations remain elusive. For instance, while ionization energies might be linked to the electronic characteristics of inter-atomic bonding in SMAs, this relationship is not definitively causal. Similarly, the correlation with the Voronoi coordination number could be attributed to its relation to the atomic radius in a given environment, which may influence crystal lattice distortion and, consequently, the compatibility at austenite and martensite interfaces. However, caution must be taken to avoid over-interpreting these assumptions. The transformation behavior in SMAs is inherently complex, making it challenging to

distill a straightforward, satisfactory physical explanation for these observations. The identified correlations are evident, yet the multifaceted nature of SMA behavior warrants a cautious and nuanced interpretation of these statistical relationships.

3.2. Correlation with thermodynamic parameters

The λ_2 parameter is instrumental in determining the expected range of hysteresis during the transformation of a given SMA. Notably, values approaching 1 typically indicate a propensity towards lower hysteresis [39–41]. However, proximity to 1 is not a definitive guarantee of reduced hysteresis. This trend is evident in Fig. 4.a, where a gradual decrease in hysteresis is observed with values nearing 1. This observed trend is also clearly evident in the super feature, as illustrated in Fig. 4.b. This figure demonstrates that alloys with an avg_first_ion_en_divi_voro_coord value near 0.7 eV exhibit reduced thermal hysteresis. Nonetheless, for a given λ_2 value, the hysteresis can vary due to a multitude of factors. These include variations in processing parameters and the specific type of martensite that may form [6,20,72,126]. Hysteresis seems to show a stronger correlation with latent heat, as depicted in Fig. 5; however, employing latent heat as a design parameter in models presents a significant challenge due to the necessity of its measurement. Such nuances highlight the complexity and intricacies involved in predicting hysteresis in NiTi alloy systems.

In our analysis of other thermodynamic parameters (Fig. 6), we observed correlations between both λ_2 and avg_first_ion_en_divi_voro_coord with M_s and θ_c . The correlation with M_s aligns with the findings presented in Frenzel et al. (2015) [10]. However, while Bucsek et al. (2016) [44] reported no significant correlation between θ_c and λ_2 , our data in Fig. 6.c suggests some observable trends. Despite literature suggestions [10], our study did not find meaningful trends between

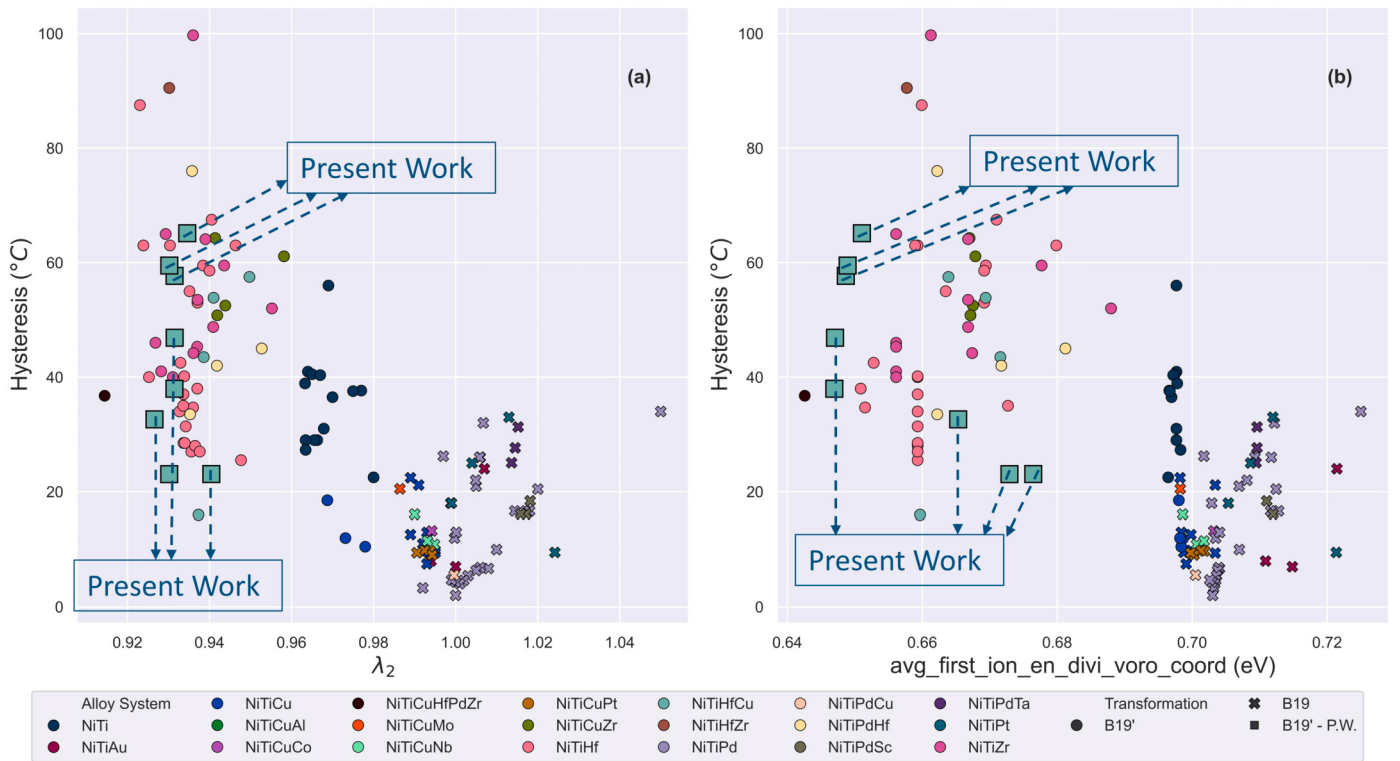


Fig. 4. The trend between hysteresis and parameters (a) λ_2 , and (b) $\text{avg_first_ion_en_divi_voro_coord}$.

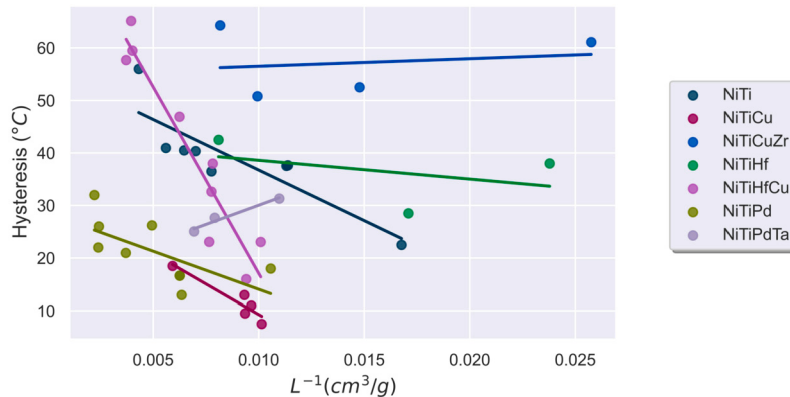


Fig. 5. The trend between hysteresis and L .

enthalpy and either λ_2 or $\text{avg_first_ion_en_divi_voro_coord}$. This discrepancy may be attributed to an insufficient data set, which could impede the emergence of significant trends.

4. Summary and conclusions

The paper illustrates the usefulness of data-driven methodologies for exploring the complex search space of SMAs and discovering novel alloys with enhanced functional properties. In this work:

- An interpretable empirical model was developed that predicts the phase compatibility of NiTi-based SMAs based on their composition. The model uses a piecewise linear regression approach to estimate the λ_2 parameter, which reflects the degree of compatibility between the austenite and martensite phases. The model also identifies the type of martensitic transformation ($B19$ or $B19'$) for a given alloy.
- The model is validated by experimental data from various literature sources and in-house measurements, showing good agreement

with the observed values. The model also provides insights into the underlying relationships between the compositional features, the λ_2 parameter and the hysteresis.

- The model identifies the weighted average of the quotient of the first ionization energy and the Voronoi coordination number as a key compositional characteristic that influences the phase compatibility and thermal hysteresis of NiTi-based SMAs. This discovery underscores the significance of atomic size mismatch and electronegativity in the formation of $B19$ or $B19'$ martensitic structures. However, it is essential to exercise caution to prevent over-interpretation of these correlations.

Declaration of generative AI in scientific writing

ChatGPT 4 and GrammarlyGO were used to brainstorm and refine sentence structures in select parts of the manuscript. The author(s) fully reviewed and revised these sections, taking complete responsibility for the final content.

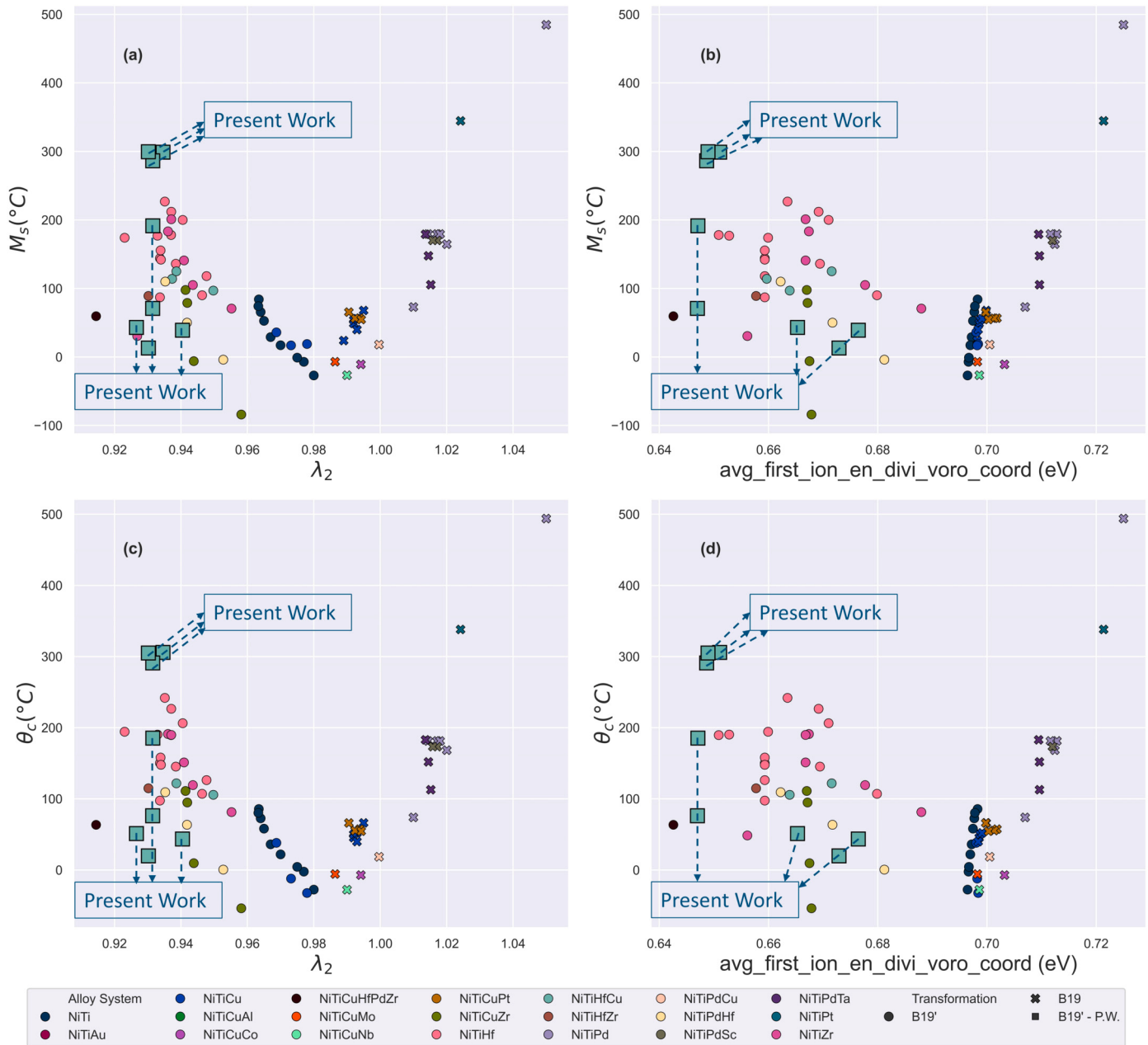


Fig. 6. Correlation analysis between martensitic transformation temperatures and key parameters: This set of subplots elucidates the relationships between M_s and θ_c , and the parameters λ_2 and $\text{avg_first_ion_en_divi_voro_coord}$.

CRediT authorship contribution statement

Sina Hossein Zadeh: Writing – original draft, Visualization, Validation, Software, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **Cem Cakirhan:** Resources, Investigation. **Daniel Khatamsaz:** Writing – review & editing, Resources. **John Broucek:** Investigation. **Timothy D. Brown:** Writing – review & editing, Resources. **Xiaoning Qian:** Writing – review & editing, Conceptualization. **Ibrahim Karaman:** Writing – review & editing, Conceptualization. **Raymundo Arroyave:** Writing – review & editing, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data and code availability

This research's dataset and source code are publicly accessible in the following GitHub repository: <https://github.com/sinazadeh/Phase-Compatibility-Model-NiTi>.

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