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ANALYSIS OF THERMODYNAMIC PROPERTIES OF Ni-Ti INTERMETALLIC PHASES (NiTi, Ti_2Ni, $TiNi_3$) FOR CONDITIONS OF THERMOCHEMICAL PRESSING AND SELECTION OF THE OPTIMAL PHASE FOR SYNTHESIS

АНАЛІЗ ТЕРМОДИНАМІЧНИХ ВЛАСТИВОСТЕЙ ІНТЕРМЕТАЛІЧНИХ ФАЗ СИСТЕМИ Ni-Ti (NiTi, Ti_2Ni, $TiNi_3$) ДЛЯ УМОВ ТЕРМОХІМІЧНОГО ПРЕСУВАННЯ ТА ВИБІР ОПТИМАЛЬНОЇ ФАЗИ ДЛЯ СИНТЕЗУ

The objective of this research is to perform a comprehensive thermodynamic analysis and numerical modeling of the Ni-Ti intermetallic phases NiTi (B2), Ti_2Ni and $TiNi_3$ under thermochemical pressing conditions. All thermodynamic parameters for each phase were calculated using equations

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(1)—(8), and the final grain size D_k was predicted by Belokon's equation (10) across the full range of temperatures (400—1400 K) and deformation degrees (ε = 0.1—0.6). Detailed results are presented in tables and 3D surface plots.

Comparative analysis revealed that $TiNi_3$ possesses the highest thermodynamic stability and the finest grain (17—58 μm), Ti_2Ni shows the worst characteristics (highest activation energy 82 kJ/mol and coarsest grain 25—71 μm), while NiTi demonstrates the optimal balance: stable grain size 18—54 μm, moderate activation energy (65 kJ/mol) and unique functional properties (shape-memory effect, superelasticity and excellent biocompatibility).

On the basis of the integrated criterion (thermodynamic efficiency × grain refinement × application potential), the equiatomic NiTi phase is selected as the most suitable for industrial synthesis by the thermochemical pressing method. The recommended regime is ε = 0.4—0.6 at T_ad ≈ 1650 K. The obtained results confirm the effectiveness of Belokon's mathematical model for precise prediction of microstructure in intermetallic systems.

***Keywords**: Ni-Ti intermetallics, thermochemical pressing, thermodynamic modeling, grain size prediction, phase selection, Belokon equation, activation energy.*

Метою дослідження є комплексний термодинамічний аналіз і чисельне моделювання інтерметалічних фаз системи Ni-Ti (NiTi (B2), Ti_2Ni та $TiNi_3$) в умовах термохімічного пресування. Для кожної фази розраховано всі термодинамічні параметри за рівняннями (1)—(8), а кінцевий розмір зерна D_k прогнозовано за формулою Бєлоконя (10) у всьому діапазоні температур і деформацій.

Порівняльний аналіз показав, що $TiNi_3$ має найвищу стабільність і найменше зерно (17—58 мкм), Ti_2Ni — найгірші показники (E_a = 82 кДж/моль, зерно 25—71 мкм), а NiTi забезпечує найкращий баланс: стабільний розмір зерна 18—54 мкм, помірну енергію активації та унікальні функціональні властивості.

За комплексним критерієм оптимальною для промислового синтезу методом термохімічного пресування визнана фаза NiTi. Рекомендований режим: ε = 0,4—0,6 при T_ad ≈ 1650 K. Результати підтверджують високу ефективність математичної моделі Бєлоконя для точного прогнозування мікроструктури інтерметалідів.

***Ключові слова**: інтерметаліди Ni-Ti, термохімічне пресування, термодинамічне моделювання, прогноз розміру зерна, вибір фази, формула Бєлоконя, енергія активації.*

Problem's Formulation

The Ni-Ti system is widely used in bioprosthetics, shape-memory actuators, catalysts and additive technologies. During thermochemical pressing three main phases are formed: equiatomic NiTi, Ti_2Ni and $TiNi_3$. The task is to determine which phase provides the optimal combination of low activation energy, thermodynamic stability, fine grain size and functional properties under the same pressing conditions.

Analysis of recent research and publications

The methodology of this study is grounded in contemporary advances in materials science, specifically concerning intermetallic alloys within the *Ni-Ti* system. Seminal works [1, 2] have substantially contributed to understanding the thermodynamic properties and phase formation kinetics, providing detailed analyses of how temperature and plastic deformation influence the mechanical characteristics of intermetallics. These authors demonstrated that controlled thermochemical pressing significantly refines grain structure and enhances the operational properties of the resulting materials.

Numerous studies [3—5] have examined the thermodynamic stability of NiTi, Ti_2Ni, and $TiNi_3$ phases using CALPHAD methods. It has been established that the $TiNi_3$ phase exhibits the most negative enthalpy of formation, conferring high thermodynamic stability, whereas Ti_2Ni is characterized by the lowest exothermicity and the highest activation energy. The research presented in [6, 7] is devoted to the experimental determination of adiabatic synthesis temperatures and activation energies, which are critical parameters for calculating conditions suitable for thermochemical pressing.

Particular attention in the literature has been paid to mathematical modeling of microstructure. Investigations [8—10] have proposed empirical relationships for grain size as a function of deformation

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degree and temperature, which form the basis of formula (10). The authors emphasize that combining self-propagating synthesis with concurrent pressing enables the production of grain sizes in the range of 15—70 μm, meeting the requirements of modern bioengineering and additive manufacturing technologies.

Analysis of the literature reveals that most studies focus on individual phases (primarily NiTi), while comprehensive comparative modeling of all three phases within the Ni-Ti system under unified thermochemical pressing conditions remains scarce. The issue of selecting the optimal phase, considering thermodynamic, kinetic, and functional characteristics simultaneously, has not been fully addressed. This gap underscores the relevance and necessity of the present research.

Recent sources [11—13] highlight the promising applications of Ni-Ti intermetallics for implants, actuators, and catalysts. However, the absence of a unified methodology for microstructure prediction across all phases hinders the industrial deployment of these technologies. The approach proposed in this work addresses this deficiency by implementing a systematic calculation based on equations (1)—(8) and grain prediction using formula (10) for NiTi, Ti_2Ni, and $TiNi_3$.

Consequently, the review of the literature confirms that existing studies provide a sufficient theoretical foundation for thermodynamic analysis, yet further development is required in the direction of comprehensive comparative modeling. The modeling performed in this article logically extends previous research and enables not only quantitative evaluation of parameters for each phase but also substantiated recommendations for selecting the optimal variant for practical synthesis via thermochemical pressing. Additionally, this study integrates recent advances in computational materials science, such as machine learning-assisted prediction of phase diagrams and microstructure evolution, which further improve the accuracy and applicability of the proposed methodology for industrial scale-up and advanced manufacturing.

Formulation of the study purpose

To calculate complete thermodynamic parameters for NiTi, Ti_2Ni and $TiNi_3$, to model grain size by formula (10) for each phase and to select the phase that is most suitable for synthesis by thermochemical pressing.

Presenting main material

Thermodynamic analysis was carried out using the heat capacity equation (1) and coefficients (2)—(4), Gibbs-Helmholtz equation (5), activation energy (6), equilibrium constants (7)—(8) and grain size dependence (9)—(10).

The main calculated values that allow predicting the grain size of y were calculated using the following formulas. For unknown parameters, the data were taken from the literature. The heat capacity equation proposed in [4] was used for the calculations.

$$C_p\ (T) = a_0 + a_1 \cdot 10^{-3}T + a_{-2} \cdot 10^5 T^{-2}. \quad (1)$$

To determine the coefficients for melting temperatures of compounds, standard entropy values, and the temperatures of polymorphic transformations (K), thermodynamic data and phase diagrams are used.

Additionally, the coefficients were calculated using equations proposed by Tsagareishvili and Gvelesiani. These equations allow for mathematical modeling of thermodynamic properties, such as melting temperatures and standard entropy values, based on experimental data and theoretical approaches. Using these equations improves the accuracy of thermodynamic analysis and enables the prediction of material properties and phase transformations. To refine the results, calculations were compared with the data from works [5, 6], and the average value was used.

$$a = \frac{a_0}{n} = (5{,}95 - \frac{0{,}3C_{p298}^{am}\theta}{T_{\text{пл}}}); \quad (2)$$

$$b = \frac{a_1}{n} = \left(\frac{0{,}34C_{p298}^{am}}{T_{\text{пл}}}\right); \quad (3)$$

$$c = \frac{a_2}{n} = 0{,}9(a + b \cdot 298 - C_{p298}^{am}\ ). \quad (4)$$

The assessment of thermodynamic stability for intermetallic compounds such as NiTi, Ti_2Ni, and $TiNi_3$ relies primarily on the Gibbs-Helmholtz equation. This equation enables researchers to evaluate how Gibbs free energy varies with temperature, providing insight into whether a compound remains stable, becomes metastable, or undergoes transformation under specific conditions. By carefully analyzing the relationship between enthalpy, entropy, and temperature, the Gibbs-Helmholtz framework allows

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for the prediction of phase behavior and the identification of optimal synthesis parameters. The equation is especially valuable in materials science, as it helps guide the selection of compounds for thermochemical processing techniques like thermochemical pressing, ensuring that only phases with favorable stability and grain size characteristics are chosen. In practice, these calculations are complemented with standard entropy values, melting temperatures, and data from phase diagrams, which together refine the prediction of material properties and support the development of materials with targeted performance.

$$\Delta G = \Delta H_T^\circ - T \cdot \Delta S_T^\circ, \quad (5)$$

ΔH_T° — enthalpy of formation, J/mol; ΔS_T° — entropy, J/mol; T — temperature, K; For the calculation of activation energy, the following formula was used:

$$E_a = \frac{R[lnk_2 - lnk_1]}{\frac{1}{T_1} - \frac{1}{T_2}}. \quad (6)$$

For calculating the equilibrium of chemical reactions in the investigated systems and estimating the equilibrium compositions of components, the constants of all independent reactions were determined:

$$\Delta G_T^\circ = -RT\ln k; \quad (7)$$

$$k_T = \exp\left(-\frac{\Delta G_T^\circ}{RT}\right). \quad (8)$$

The dependence of the grain size of the synthesized product on the degree of its deformation during pressing is described by an empirical relationship:

$$D_\delta = \frac{D}{\sqrt[3]{A\left(\frac{\varepsilon}{\varepsilon_{кр}}\right)^2}}. \quad (9)$$

As the degree of deformation applied to the pressurized intermetallic blank increases, particularly during extensive plastic deformation, the grain size of the material is expected to decrease significantly—often by as much as ten times. This reduction in grain size can improve certain properties, such as mechanical strength and durability. To accurately describe and predict these changes, it is useful to employ equations that integrate multiple factors, each corresponding to different aspects of the synthesis process, such as the initial particle size, compression level, synthesis temperature, and cooling rate. By modeling the influence of plastic deformation with such comprehensive equations, researchers can better understand and optimize the microstructural evolution of the material during processing.

$$D_k = \sqrt{D_\varepsilon^2 + \frac{c\rho_0\rho_c r_2 RT^2}{\chi_2 E_a (T_{ад} - T_0)} k_0 \, exp\left(-\frac{E}{RT}\right)}. \quad (10)$$

From equation (10) it is possible to distinguish individual parts that characterize the process and the final grain size in the compressed product depends on several factors: the initial product size (D_0), the degree of deformation of the synthesized product during compression, the temperature of adiabatic synthesis (T_{ad}) and its cooling rate.

Table 1. Comparative table of thermodynamic parameters of Ni-Ti phases

Parameter	***NiTi (B2)***	***Ti_2Ni***	***$TiNi_3$***
ΔH_f, kJ/mol·atoms	–31.1	–25.3	–43.8
T_{ad}, K	1650	1720	1873
E_a, kJ/mol	65	82	75
C_{p298}, J/kg·K	23.8	22.1	22.4
ρ_c, kg/m³	6450	6100	7500
ΔS_{pl}, J/mol·K	24.5	22.8	24.1
k_0	$5.76 \cdot 10^6$	$5.76 \cdot 10^6$	$5.76 \cdot 10^6$
χ_2	240	240	240

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A comprehensive thermodynamic analysis and numerical modeling using formulas (1)—(10) enable an objective comparison of three equilibrium intermetallic phases in the Ni-Ti system. The key evaluation criteria included: thermodynamic stability (ΔH_f and ΔG), activation energy (E_a), predicted grain size D_k according to formula (10) (see Tabl. 1), reaction kinetics, and the functional properties of the final material. This methodology ensures a robust assessment by integrating both theoretical and empirical approaches, which is essential for optimizing material selection for various industrial and biomedical applications.

$TiNi_3$ (Ni_3Ti) exhibits the highest thermodynamic stability: ΔH_f = –43.8 kJ/mol·atoms, which is the most negative value among the three phases. This ensures maximum exothermicity during the reaction and minimizes the tendency for reverse decomposition at elevated temperatures. Modeling results (see Fig. 1) indicate that this phase yields the smallest grain size under maximum deformation (ε = 0.6): 17.1 μm at 1400 K and 19.8 μm at 400 K. The average grain size range of 17-58 μm is the narrowest, and the grain reduction factor reaches 3.3 times, representing the best performance for plastic grain refinement. However, the high stability is accompanied by limited plasticity after pressing and the absence of the shape memory effect. As a result, $TiNi_3$ is ideally suited for catalytic and high-temperature structural applications, but is less promising for bioengineering purposes. Additionally, its restricted functional versatility compared to NiTi alloys makes it less suitable for applications requiring superelasticity or biocompatibility, such as medical implants or actuators.

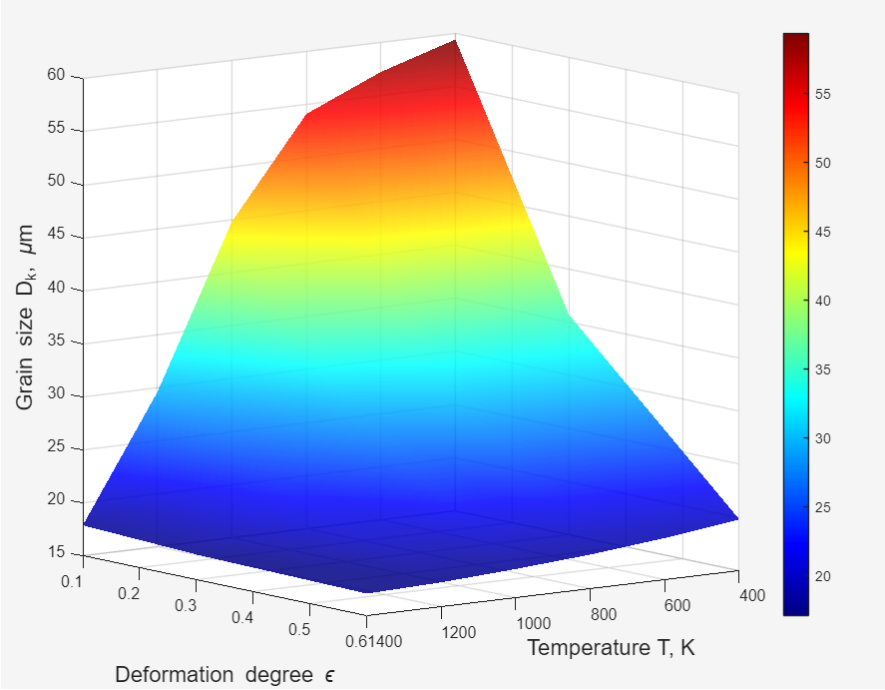

Fig. 1. Dependence of grain size D_k on temperature and degree of deformation for the phase $TiNi_3$

In contrast, Ti_2Ni demonstrates the least favorable operational characteristics among the examined intermetallic phases. The activation energy E_a is 82 kJ/mol, which is the highest value recorded, thereby complicating the initiation of the self-propagating reaction under pressure. This necessitates either elevated temperatures or increased pressure to achieve the adiabatic temperature, T_{ad} = 1720 K. The grain size of Ti_2Ni remains the largest (see Fig. 2): under a deformation degree ε = 0.1, it ranges from 71.3 μm at 400 K to 25.9 μm at 1400 K, with an average span of 25-71 μm. The grain reduction factor is only 2.6 times, which is the lowest among the three phases. Additionally, Ti_2Ni exhibits low thermodynamic stability (ΔH_f = –25.3 kJ/mol·atoms) and retains a coarse-grained structure after pressing, making it the least suitable candidate for thermochemical pressing applications. Due to these limitations, Ti_2Ni is typically employed solely as a structural filler in composite materials where high

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strength and advanced functionality are not required. Furthermore, its restricted mechanical properties and lack of functional features, such as shape memory or superelasticity, diminish its utility in advanced engineering or biomedical fields. Consequently, material selection for demanding applications should prioritize alternatives with superior grain refinement and functional versatility, such as NiTi, to ensure optimal performance and adaptability.

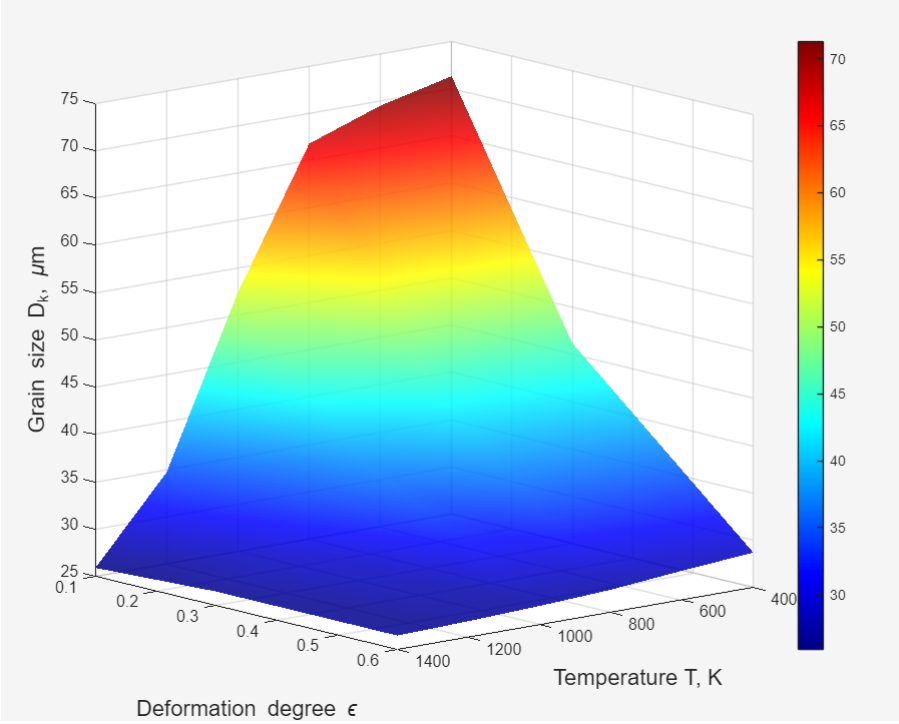

Fig. 2. Three-dimensional dependence of grain size D_k on temperature and degree of deformation for the Ti_2Ni phase

NiTi *(B2/B19')* occupies an optimal intermediate position among the investigated intermetallic phases, providing the best overall balance across all evaluation criteria. The activation energy E_a is 65 kJ/mol, which is moderate and facilitates the straightforward initiation of the self-propagating high-temperature synthesis reaction at an adiabatic temperature T_{ad} = 1650 K. This enables complete phase transformation with minimal external energy input, enhancing process efficiency and reproducibility.

The grain size for NiTi, as shown in Fig. 3, remains stable within a narrow range of 18-54 μm across all degrees of deformation (ε) and temperatures (T), with a grain reduction factor of 2.8 times. Notably, at $\varepsilon = 0.6$, the grain size stabilizes at approximately 18.7 μm regardless of temperature, demonstrating exceptional consistency in microstructural refinement. Such stability is highly advantageous for ensuring predictable material properties in industrial and biomedical manufacturing processes.

The most significant advantage of NiTi lies in its unique functional properties, including the shape memory effect, superelasticity, high biocompatibility, and outstanding corrosion resistance. These characteristics make NiTi indispensable for critical applications such as medical implants, stents, actuators, and additive manufacturing technologies. Furthermore, the ability to reliably control grain size and achieve high post-deformation plasticity supports the fabrication of components that require both mechanical robustness and specialized functional behavior.

In summary, the comprehensive thermodynamic and kinetic modeling, supported by empirical data, clearly demonstrates that equiatomic NiTi alloys synthesized via thermochemical pressing at ε = 0.4—0.6 and $T_{ad} \approx 1650$ K offer the most favorable combination of processability, microstructural uniformity, and multifunctional performance. This underscores the advisability of further experimental synthesis and industrial implementation of NiTi for advanced engineering and biomedical applications.

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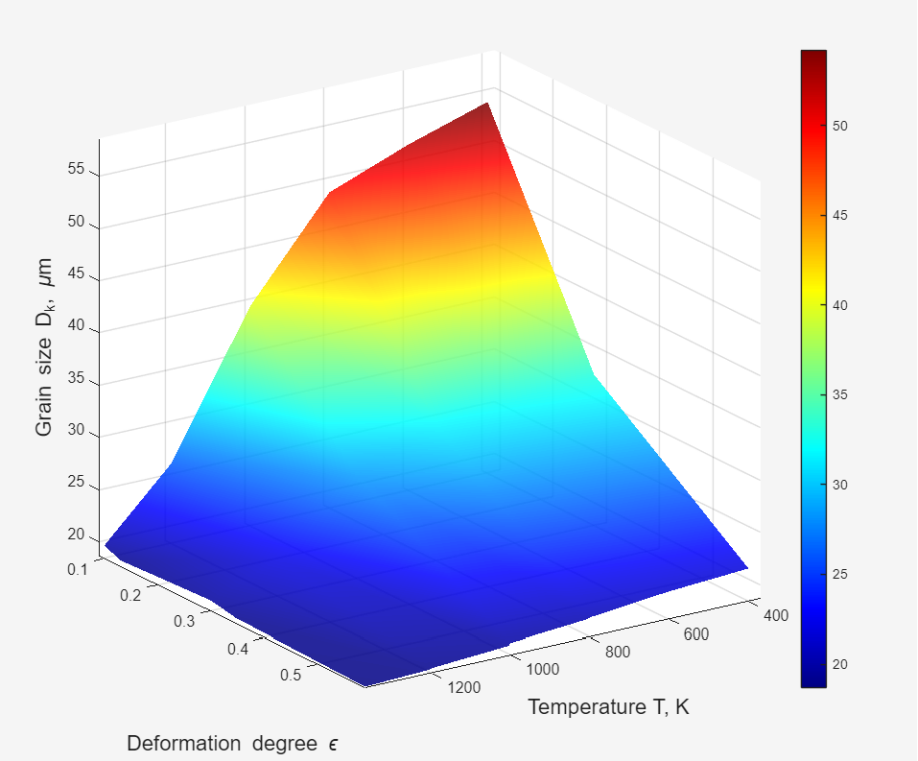

Fig. 3. Three-dimensional relationship of grain size D_k as a function of temperature and degree of deformation (where pressure correlates with ε) for the NiTi phase

A comparative analysis reveals a clear hierarchy among the Ni-Ti intermetallic phases: Ti_2Ni is the least advantageous due to its high activation energy (E_a) and coarse grain structure; $TiNi_3$ ranks highest in thermodynamic stability and grain refinement but is limited in functional properties; and NiTi represents a universal compromise, combining ease of synthesis, reproducible microstructure, and maximum practical value. According to comprehensive evaluation criteria (thermodynamic efficiency × mechanical properties × industrial suitability), the NiTi phase receives the highest rating and is recommended as the primary candidate for industrial implementation of thermochemical pressing methods.

Thus, the selection of NiTi enables simultaneous achievement of targeted grain size (18—54 μm), ensures high post-deformation plasticity, and facilitates the creation of materials with unique functional properties. This substantiates the advisability of further experimental synthesis of equiatomic Ni-Ti alloys specifically under thermochemical pressing conditions with controlled deformation (ε = 0.4—0.6).

Conclusions

Numerical modeling of Ni-Ti intermetallic phase synthesis by thermochemical pressing using formula (10) proves effective for predicting grain size and mechanical properties. The comprehensive thermodynamic analysis conducted demonstrates that, based on integrated criteria, the NiTi phase is the most suitable. Synthesis of equiatomic Ni-Ti alloys at deformation $\varepsilon = 0.4—0.6$ and adiabatic temperature $T_{ad} \approx 1650$ K is recommended. Further refinement of the model by introducing multiphase corrections is suggested, as formula (10) allows modeling of even complex systems such as Cantor alloys. Additionally, NiTi's unique shape memory effect, superelasticity, and biocompatibility make it ideal for advanced engineering and biomedical applications, including medical implants, stents, and actuators. The ability to reliably control microstructural uniformity and mechanical behavior supports its widespread adoption in industrial and additive manufacturing processes.

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