Metallurgical and Materials Data 1, no. 1 (2023): 1-6

Publisher: Association of Metallurgical Engineers of Serbia

Metallurgical and Materials Data

www.metall-mater-data.com

Titanium alloys database for medical applications

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ARTICLE INFORMATION:

https://doi.org/10.30544/MMD5

Received: 27 March 2023
Accepted: 30 March 2023

Type of paper: Database description

Database URL: https://doi.org/10.5281/zenodo.7802694

ABSTRACT

Titanium alloys are widely applied, particularly in biomedical engineering, due to their exceptional combination of mechanical strength, corrosion resistance, and biocompatibility. The low modulus of elasticity of these titanium alloys in comparison to other materials used in medical applications is a main characteristic. However, some of these alloys' components, such as aluminum and vanadium, can have adverse effects on the human body. Consequently, new titanium alloys with low modulus of elasticity and no toxic alloying elements are currently being developed. In this research, 238 titanium alloys were collected, almost entirely composed of biocompatible alloying elements. The primary motivation behind creating such a database is to establish a foundation for designing new alloys using machine learning methods. The database can assist researchers, engineers, and biomedical professionals in developing titanium alloys for various medical applications, thereby improving health outcomes and driving advancements in biomaterials and biomedical engineering.

Keywords: Titanium Alloys Database; Biocompatible; Medical Applications; Biomedical; Non-Toxic Elements.

1. Introduction

Titanium alloys are categorized as critical materials in medical applications due to their unique properties, including biocompatibility, corrosion resistance, and mechanical strength. They are widely applied in orthopedic implants, prosthetic hips, and joint prostheses (Liang et al. 2020, Sidhu et al. 2021). These materials must withstand the hostile environment of the human body, where they are exposed to a corrosive environment with a pH of approximately 7 and daily bone stress levels of approximately 4 MPa (Eliaz, 2019). The average load on a healthy hip joint can reach up to three times a person's body weight (up to 3000 N), and extreme loads during a jump can reach up to ten times the body weight (Moghadasi et al. 2022, Cleather et al. 2013, Tanikić et al. 2012). Material fatigue can result from both the constant stress of the human body weight and the cyclic stress caused by friction between metal implants and bones. This friction leads to a reduction in the oxide layer's viability, surface damage, and the formation of free metal surfaces. An initial crack in the metal can be caused by friction and corrosion of the free metal surface. When this crack reaches a critical size under the present stress, it can rapidly propagate and lead to implant failure. In the human body, the friction of metal materials leads to the continuous release of metal ions, compounds, and wear products (Eliaz, 2019, Prasad et al. 2017). This demonstrates the potential for the human body to decompose metal implants, resulting in decreased durability due to chemical and mechanical stresses. Additionally, the release of toxic alloying elements from these implants can spread throughout the body, leading to various health issues (Davis et al. 2022, Markowska-Szczupak et al. 2020, Liang 2020). The toxicity of elements, including metals, is largely determined by their concentration in the human body; even bio-elements can become toxic if their recommended levels are exceeded. When evaluating the biocompatibility and bioactivity of metal-based medical materials, it is critical to consider concentration-dependent toxicity, as the activity of certain ions can vary depending on their concentration in the medium (Milojkov et al., 2023). In the literature, the following alloying elements are considered toxic in titanium alloys: Pt, Al, V, Ni, Co, Cu, and Cr (Eliaz, 2019).

The need for a comprehensive database of titanium alloys for medical applications arises from the existing challenges in selecting suitable alloys that meet specific requirements regarding biocompatibility and mechanical properties. With many titanium alloys developed for biomedicine, it's crucial to identify alloys that possess good mechanical properties, have a modulus of elasticity close to that of bone (10 to 30 GPa), and avoid toxic alloying elements. One widely used alloy, Ti-6Al-4V, has shown long-term clinical issues due to the presence of aluminum and vanadium, which can cause harmful effects on the human body. To address this, researchers are investigating biocompatible elements, such as Ti, Nb, Zr, Ta, Ru, and Sn, to be included in new alloy designs.

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Nonetheless, the cost of these components must be considered during the design of new materials. Employing porosity in metallic biomaterials can be advantageous, as it not only enhances biocompatibility but also reduces the modulus of elasticity, leading to better stress distribution and improved implant performance (Bandyopadhyay et al. 2022).

There are open-access databases available, such as MatWeb Titanium Alloy Property Data (MatWeb 2023), but they do not specifically focus on biocompatible alloys (over 390 titanium alloys). Currently, there is a newer open-access database named "A compilation of experimental data on the mechanical properties and microstructural features of Ti-alloys," with about a 7% overlap with our database (Salvador et al. 2022). This database also includes toxic alloying elements, such as Al and V. Some researchers have reported employing databases for machine learning research, but the databases themselves have not been made public. For instance, Zou et al. 2021 reported on 41 binary and 81 multicomponent Ti-alloys in their study. On the other hand, Wu et al. conducted comprehensive research on phase stability prediction using machine learning methods, where they collected 292 data points from 63 studies (Wu et al., 2022), and presented 112 data points in their earlier paper (Wu et al., 2020) for the following elements: Ti, Nb, Zr, Sn, Mo, and Ta.

The objective of creating a titanium alloy database for medical applications is to provide a centralized, accessible, and comprehensive source for data on titanium alloys, connecting their composition with mechanical properties and biocompatibility. The creation of such a database is essential for the design of new titanium alloys, as it enables researchers to effectively employ a variety of methods and principles. This includes the Mo equivalent method, the electron-to-atom ratio (e/a) method (Tiwari and Ramanujan, 2001), the alloy design method based on d electrons (Song et al. 2000), experimental techniques (Zhu et al. 2021, Ehtemam-Haghighi et al. 2017), and finally using the machine learning methods (Xiong et al. 2020, Wu et al. 2020, 2022). The database enables researchers to optimize alloy design by considering the effects of different alloying elements, and mechanical and heat treatment on mechanical properties. Such a database streamlines the titanium alloy design process, allowing for more effective development of biomedical materials.

2. Methods

2.1. Data Sources and Collection Methods

The data sources for the database consist of high-quality, peer-reviewed research papers, which were manually selected by the authors. The primary criterion for including titanium alloys in the database was their alloy composition, with a focus on non-toxic elements. Also, other elements are considered, as shown in the next sub-chapter. The non-toxic elements considered for the database include:

Biocompatible elements: Nb, Zr, Ta, Ru, Sn;
Neutral elements: Fe, Mn, Si, W, Hf, Mo;
Alloy inclusions: O, N, C.

The database has been uploaded to the open-source platform Zenodo, which is a suitable platform for preserving and updating the database. Currently, 238 biocompatible titanium alloys have been collected.

To ensure the accuracy of the data, the authors have checked the information three times, and the dataset will be subjected to peer review alongside this manuscript. While the research papers used as data sources are peer-reviewed and considered credible, there is still a possibility that some data may be unreliable. If any unreliable data is confirmed by other peer-reviewed papers, the database on the Zenodo platform will be updated accordingly with the corrected information.

2.2. Database Structure and Organization

The database structure for titanium alloys used in medical applications consists of several columns, each providing specific information about the alloy:

1. "Sort": Facilitates alphabetical sorting based on alloying element content (from highest to lowest), with a number representing the rounded amount of the first alloyed element (datatype: string).
2. "Reference": Contains the source data cited in this paper's references (datatype: string).
3. "Material": Refers to the content of alloying elements and alloy designation from the source paper (datatype: string).
4. "Product": Indicates the manufacturing method of the alloy (datatype: string, missing data: 91).
5. "Mechanical treatment": Specifies the mechanical treatment applied to the alloy (datatype: string, missing data: 169).
6. "Deformation, %": Shows the degree of deformation after mechanical treatment (datatype: real number, missing data: 176).
7. "Heat treatment": Describes the heat treatment for the alloy (datatype: string, missing data: 115).
8. "HT1: T, C": Provides data for the temperature (in Celsius) of the first heat treatment (datatype: real number).
9. "HT1: t, min": Gives data for the duration (in minutes) of the first heat treatment (datatype: integer).
10. "HT2: T, C": Provides data for the temperature (in Celsius) of the second heat treatment (datatype: real number).
11. "HT2: t, min": Gives data for the duration (in minutes) of the second heat treatment (datatype: integer).

Columns 12-42 contain alloy composition data (first at.%, followed by wt.%) for each element: Ti, Nb, Zr, Ta, Sn, Fe, Mn, Si, V, Mo, Cu, Cr, O, N, C (datatype: real number).

43. “Module last, exp, GPa”: Experimentally determined value of modulus of elasticity (or Young's modulus) of the alloy (datatype: real number, no missing data).
44. “±d(GPa)”: Deviation from the experimentally determined value of modulus of elasticity (or Young's modulus) of the alloy (datatype: real number).
45. “Elongation, %”: Experimentally determined value for elongation (in %) of the alloy (datatype: real number, missing data: 142).
46. “Max Tensile strength (MPa)”: Experimentally determined value for tensile strength (in MPa) of alloy (datatype: real number, missing data: 136).
47. “Yield strength (MPa)”: Experimentally determined value for yield strength (in MPa) of the alloy (datatype: real number, missing data: 138).
48. “Hardness (HV)”: Experimentally determined value for hardness (in HV) of the alloy (datatype: real number, missing data: 193).
49. Density”: Calculated density of the alloy using the formula:

$$D = \sum_{1}^{n} m_i D$$

Where m_i is atomic weight, and D is the density of the nth element in the alloy (datatype: real number).

50. “e/a ratio”: Electron-to-atom ratio, calculated using the formula:

$$e / a = \sum_{1}^{n} a_i V_i$$

Where, V_i is the total number of valence electrons in the valence shell, and a_i is the atomic percentage of the n^th^ element in the alloy (datatype: real number).

51. "[Mo]eq_B": Represents the Mo equivalent according to the reference, calculated using a specific equation provided in the reference (Liang 2022):
    [Mo]eq_B = Mo + 0.67 V + 0.44 W + 0.28 Nb + 0.22 Ta + 2.9 Fe + 1.6 Cr + 0.77 Cu + 1.11 Ni + 1.43 Co + 1.54 Mn + 0.0 Sn + 0.0 Zr - 1.0 Al (wt.%)
    (Datatype: real number).
52. "[Mo]eq_Z": Represents the Mo equivalent according to the reference, calculated using a specific equation provided in the reference (Liang 2022):
    [Mo]eq_Z = Mo + 0.74 V + 0.5 W + 0.39 Nb + 0.28 Ta + 2.2 Fe + 1.69 Cr + 0.85 Cu + 1.22 Ni + 1.57 Co + 1.69 Mn + 0.0 Sn + 0.0 Zr - 1.0 Al (wt.%)
    (Datatype: real number).
53. "[Mo]eq_W1": Represents the Mo equivalent according to the reference, calculated using a specific equation provided in the reference (Liang 2022):
    [Mo]eq_W1 = Mo + 1.25 V + 0.59 W + 0.28 Nb + 0.22 Ta + 1.93 Fe + 1.84 Cr + 1.51 Cu + 2.46 Ni + 2.67 Co + 2.26 Mn + 0.3 Sn + 0.47 Zr + 3.01 Si - 1.47 Al (wt.%)
    (Datatype: real number).
54. "[Mo]eq_W2": Represents the Mo equivalent according to the reference, calculated using a specific equation provided in the reference (Liang 2022):
    [Mo]eq_W2 = Mo + 0.74 V + 1.01 W + 0.23 Nb + 0.3 Ta + 1.23 Fe + 1.1 Cr + 1.09 Cu + 1.67 Ni + 1.81 Co + 1.42 Mn + 0.38 Sn + 0.34 Zr + 0.99 Si - 0.57 Al (wt.%)
    (Datatype: real number).
55. "Bo - bond order": The Bond order, calculated using the formula:

$$Bo = \sum_{1}^{n} m_i Bo_i$$

Where m_i is atomic weight, and Bo_i is the bond order of the n^th^ element in the alloy (datatype: real number).

56. "d-orbital energy level ($M\bar{d}$)": d-orbital energy level, calculated using the formula:

$$M\bar{d} = \sum_{1}^{n} m_i M\bar{d}_i$$

Where m_i is atomic weight, and $M\bar{d}$ is the d-orbital energy level of the n^th^ element in the alloy (datatype: real number).

The data generated from calculations (columns 49-56) represent important parameters in material design. The additional calculated parameters can be included, as shown in the literature (Azmat et al. 2021).

3. Discussion of the database

3.1. Description of the Contents and Structure

The titanium alloy database for medical applications is designed to enable the selection and development of biocompatible titanium alloys for medical applications. The database focuses on non-toxic elements and contains key information on:

- alloy's labels with references to the source of data,
- manufacturing methods, heat and mechanical treatment processes,
- alloy compositions,
- key mechanical properties,
- and additional calculated properties.

Having alloy labels with references to the source of data is important for maintaining order and reliability in a database. Along with labeling and citing the research sources, researchers can easily follow the origins of the data and assess its credibility. As new research may reveal varying mechanical properties for alloys with the same composition in this database, depending on factors such as mechanical and heat treatments, inclusions, or testing methods, it is essential to include as many details as possible.

Manufacturing methods in this database primarily involve arc melting or selective laser melting in a vacuum or argon atmosphere. Considering the high melting points of these alloys and titanium's high affinity for oxidation, this is reasonable. Applying mechanical or heat treatments to these alloys, or different combinations of these treatments to the same alloy, can provide researchers with valuable insights into the effects of these treatments on the alloy's structure and mechanical properties. Despite a significant amount of missing data, conclusions can still be drawn about the influence of certain mechanical and heat treatments on the structure and mechanical properties of titanium alloys. However, for machine learning methods, the optimal format for presenting such data remains a topic of discussion among the broader scientific community: whether using letters or numbers to represent specific heat or mechanical processing methods is more convenient. This database contains both formats for mechanical and heat treatment, but future reorganization is possible, mainly to accommodate machine learning research methods.

The author's primary focus in the current database is on biocompatible alloying elements, as the objective is to support machine learning algorithms that recognize patterns for creating new biocompatible titanium alloys. However, other alloying elements could potentially contribute to further research using machine learning methods. Although many elements are not currently included, future expansion of the database could incorporate them. This would enable researchers to explore a wider range of titanium alloys with potential applications beyond the medical field or within specialized areas of biomedical research.

Titanium alloys are widely used as implants in the human body, and one of their most important properties is a low elastic modulus. This is necessary to minimize the "stress shielding" effect, which occurs when an implant with a significantly higher elastic modulus than the surrounding bone tissue takes over most of the load, leading to bone loss and implant loosening over time. This is the primary reason why elastic modulus is a key parameter and is included in all research studies within our database. Approximately 20% of the data in the database includes information about the deviation of the modulus of elasticity. This is highly significant for machine learning methods, as it provides insight into the reliability of the data within a specific range. Data on elongation, tensile strength, yield strength, and hardness are relatively scarce in the database. However, this information is crucial, as it is directly related to the modulus of elasticity. Moreover, these mechanical properties may be essential for meeting specific requirements in certain biomedical applications, such as load-bearing implants, dental prosthetics, or orthopedic devices.

Derived (calculated) values, such as density, e/a ratio, Mo equivalents, Bo-bond order, and d-orbital energy level, are considered some of the most important factors in titanium alloy design. To analyze the effect of most β-stabilizers, Mo equivalents ([Mo]eq) have been developed by several researchers and employed in designing new alloys (Liang 2020, Sidhu et al. 2021). For biocompatible alloys, it would be intriguing to develop new equations for Mo equivalents that could more accurately account for the β-stabilization effect of these elements. Including bond order (Bo) and d-orbital energy level (Md) in the database is important because they provide insights into the fundamental interactions between titanium and alloying elements grounded in theoretical principles. The bond order (Bo) represents the covalent bond strength between titanium and an alloying element, while the d-orbital energy level (Md) reflects the properties of transition metals as alloying elements, determined by their metallic radius and electronegativity.

3.2. Potential Biases and Limitations of the Database

The database relies on credible, high-quality, peer-reviewed research papers as its primary data source. However, there is still the possibility of unreliable data, which may impact the overall accuracy of the database. Updates may be required if issues are discovered.

Some mechanical properties, including elongation, tensile strength, yield strength, and hardness, have an insufficient number of data points in the database. This scarcity can render some methods, such as machine learning methods, impractical for application.

Although the database focuses on biocompatible elements, other elements or combinations may contribute to future research. Limiting the scope of the database to the selected elements could hinder alloy design discoveries.

Numerous factors, including mechanical and heat treatments, small amounts of inclusions, and non-standard testing procedures, can influence the mechanical properties of an alloy. It is possible that the database does not account for all these factors, which could result in data bias.

3.3. Future Directions and Expansion Database

Plans for updating and maintaining the database include:

- Regular updates: periodic updates to incorporate new research findings, ensure that the database remains relevant and current with the most recent advancements in the field of titanium alloys for medical applications.
- Encourage researchers and experts to submit new data, corrections, or updates, fostering a collaborative environment that enriches and improves the database.
- Establish a peer review procedure to evaluate the data's quality and dependability and to maintain the database's credibility.

Possible enhancements or additions to the database's structure and features:

- Expanded alloy compositions: Extend the database's scope to include additional alloying elements and their combinations.
- Enhanced treatment information: Enhance the database by adding more detailed information on mechanical and heat treatments; change the data type or reorganize it to better enable machine learning research.
- Integration with other databases or resources related to titanium alloys or medical materials.
- Including the quantitative proportion of phases (especially the beta phase) in the database as a parameter that has a direct influence on mechanical properties.
- Information regarding the concentrations of potentially toxic ions and their release from the implant, depending on the alloying elements contained in the titanium alloy, would be valuable.

4. Conclusion

The titanium alloy database for biomedical applications provides a valuable resource for researchers and professionals developing biocompatible titanium alloys for medical implants and devices. The database consolidates essential information on alloy compositions, manufacturing methods, mechanical properties, and derived key values, enabling a more systematic and efficient approach to materials research. The database has the potential to accelerate the discovery of novel materials with enhanced performance and biocompatibility by facilitating the application of machine learning methods. Plans for updating the database include regular updates, expanded functionality, and integration with other databases or resources pertaining to medical materials, ensuring its continued relevance and utility in the rapidly advancing field of materials science.

Acknowledgment

This work was supported by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Contract No. 451-03-47/2023-01/200135).

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