A compilation of experimental data on the mechanical properties and microstructural features of Ti-alloys

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The present work depicts a compilation of mechanical properties of 282 distinct multicomponent Ti-based alloys and their respective microstructural features. The dataset includes the chemical composition (in at.%), phase constituents, Young modulus, hardness, yield strength, ultimate strength, and elongation. Each entry is associated with a high-quality experimental work containing a complete description of the processing route and testing setup. Furthermore, we incorporated flags to the dataset indicating (a) the use of high-resolution techniques for microstructural analysis and (b) the observation of non-linear elastic responses during mechanical testing. Oxygen content and average grain size are presented whenever available. The selected features can help material scientists to adjust the data to their needs concerning materials selection and discovery. Most alloys in the dataset were produced via an ingot metallurgy route, followed by solubilization and water quench (≈58%), which is considered a standard condition for β-Ti alloys. The database is hosted and maintained up to date in an open platform. For completeness, a few graphical representations of the dataset are included.

Background & Summary

The number of peer-reviewed experimental investigations on the mechanical properties of Ti-alloys listed in the Web of Science exceeded four thousand five hundred (4500) in September 2021. An increasing trend in titanium research, observed over the last 30 years1, accompanies this aggregated result. Ti alloys have become essential structural materials to many industries, from aeronautical to biomedical. In the former case, their elevated strength-to-density ratio and thermal stability provide an optimal combination for the aircraft structure (skeleton) and engine parts (compressor)2. In the latter, Ti alloys are preferred candidates for bioimplants due to their low elastic modulus and superior biocompatibility, which excel most metallic systems3.

Nevertheless, even within this extensive body of research, finding a dataset that consolidates recent experimental data on Ti alloys containing multiple properties of interest has been challenging since new reports are published across a broad range of fields of study daily. While each area demands particular processing routes, testing methods, and analyses, data comparison becomes more intricate. Furthermore, different from other emerging areas in metallurgy, such as high-entropy alloys4, currently available titanium databases are either private5 or outdated6. We aim to bridge this gap by proposing a new open-source database focused on Ti alloys.

Typical experimental studies on Ti-based alloys can be divided into two groups. The first group presents analytic works, with a narrative centered on phase transformations. These works usually attain an in-depth microstructural analysis and do not report extensively on the mechanical properties7,8. On the opposite, the second group focuses on comparative analysis, which comprises a straightforward exploration of new compositions and their mechanical behavior9,10. These works tend to provide only simplistic microstructural analyses, primarily based on conventional (laboratory) X-ray diffraction. The present data article aims to establish common ground between these two initiatives. The studies compiled herein depict only well-balanced research11–13, with enough detail on both fronts (i.e., mechanical properties and microstructural features). Please check the Methods section for further information about how the papers were selected.

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The mechanical properties of Ti alloys derive from the stability and the physical traits of their phase constituents. Traditionally, the design of Ti alloys is based on tailoring the stability of equilibrium phases such as $\alpha$ (HCP, low-temperature phase) and $\beta$ (BCC, high-temperature phase), with the aid of different alloying elements. Elements named $\beta$-stabilizers (Nb, Ta, Mo, V, Fe) reduce the transition temperature between $\alpha$ and $\beta$, known as $\beta$-transus, allowing the $\beta$-phase to show at temperatures lower than 882 °C. However, processing-structure-property relationships in Ti alloys are convoluted, as the $\beta$-phase can exhibit many solid-state phase transformations upon cooling. Thus, as a reference condition, Ti-alloys are usually water-quenched (WQ) from the $\beta$-phase field, hindering diffusion-controlled transformations and promoting the retention of the prior $\beta$-phase at room temperature (RT). Exceptions to this case involve the formation of martensitic phases, such as $\alpha'$ (with hexagonal structure), $\alpha''$ (with orthorhombic structure), $\omega$-phase (also hexagonal), or active intermetallics. The $\omega$-phase is often observed in shape memory alloys and is associated with double-yielding and non-linear elastic behavior. The presence of $\omega$ is of particular concern to several applications since it can severely impair the alloy ductility.

As briefly introduced in this section, the Ti system is complex, so it is essential to gather data from previous works that report enough information on the composition, processing, microstructure, and mechanical properties. From a materials selection perspective, an open database might help with future comparative analyses, helping materials scientists to identify desired properties among known compositions. As for materials discovery, a comprehensive compilation of mechanical properties and microstructure data may allow researchers to spot unexplored regions of the vast available compositional space. Computational Materials Science works have achieved this in the past, however, due to the lack of organized experimental data, modeling and predictions were primarily performed using theoretical data obtained from first-principles calculations. The public availability of a routinely updated database will allow experimental scientists to act more proactively concerning alloy exploration.

**Method**

**Data collection.** At an initial stage, the authors selected 140 potential studies from the literature (WebOfScience, SCOPUS, ScienceDirect) based on a preliminary search using specific keywords ("titanium"; "alloys"; "ti alloys"; "mechanical properties"; "microstructure"; "experimental"). Full-texts were manually retrieved and organized, discarding studies that satisfied any exclusion criteria (next section). This dataset covers data from 1986 to 2021, with most studies being published after 2010 (approx. 84%).

We then extracted the properties of interest from each selected article and tabulated them in an online spreadsheet. Two authors worked independently at this step and registered relevant information in the comments section of each entry. In the case of studies exploring multiple compositions, each one was assigned to a single dataset record. WebPlotDigitizer was employed to extract data from graphics when needed. The three remaining authors received a random sample of 20% of the dataset for blind review as a final step. Authors only received articles they did not personally select on stage 1 for evaluation.

**Exclusion criteria.**

- absence of a compositional evaluation;
- absence of details on the processing route;
- no phase identification (minimal accepted: X-ray diffraction);
- less than two of the following mechanical properties reported: Young modulus, yield strength/ultimate strength/elongation, hardness.
- samples subjected to thermal treatments other than solution treated (ST) or stress-relief (i.e., aging, inter-critical tempering, complex heating/cooling cycles);
- for powder-metallurgy/sintered samples (f) - relative density lower than 90%.

**Blind review.** Two independent reviewers received the entry’s digital object identifier (DOI) subjected to blind review. They were also provided with a list (Table 1) containing the mechanical and microstructural features to be extracted from the text (i.e., an empty table). The reviewers independently downloaded the full text and then obtained all the variables/parameters to the best of their ability. Later, the annotated values from the two reviewers were compared with each other. In case of divergences, reviewers reach a consensus in a debate with all authors. After settling on the most appropriate number/value for the variable in question, the observations field of that entry was filled with all pertinent details on how to obtain the data - e.g. "mechanical properties extracted from Table 5", "Average grain size estimated based on Figure 7".

It is worth mentioning that blind review identified only 21 discrepancies in the dataset; 11 were approximation errors from measurements taken from images, and 10 were wrong or missing values (i.e., a value that was present in the study which was not compiled into the dataset by human error). Data readily available in text or table was always favored over data displayed in images only.

**Data Records**

The dataset consists of 282 entries obtained from 105 high-quality experimental studies. These are surviving entries from 120 articles previously selected after manual curating, filtering, and blind review. Properties in Table 1 were compiled from the original texts to the best of the authors’ abilities to interpret the published results. Some properties in this dataset, such as the oxygen content (in wppm), the average grain size, and the elongation, are compiled in an identical format to recent works. In this way, the elongation is considered positive in tensile tests and negative in compression tests. Unfortunately, not all critical properties are reported for...
all entries; this is especially problematic to address the impact of interstitial elements in Ti-alloys. Ti is highly reactive to oxygen, and minor variations in the oxygen content massively affect the phase transformations and mechanical properties. Figure 1 depicts the frequency distribution of oxygen content (wppm) and the major mechanical properties contained in the dataset. The dataset is well balanced, including a broad range of strength, ductility, and hardness values.

A widely known parameter (included in this database) to represent the $\beta$-stability is the molybdenum equivalent (MoE). In simple terms, MoE is a weighted average of the composition (Eq. 1) that combines the critical concentrations of more than ten alloying elements into a Ti-Mo binary equivalent system. According to a recent review by Kolli & Devaraj, MoE can also be used to categorize Ti-alloys into four distinct $\beta$-stability tiers: $\beta$-rich ($0 \leq \text{MoE} < 5$), near-$\beta$ ($5 \leq \text{MoE} < 10$), $\beta$-metastable ($10 \leq \text{MoE} < 30$), and $\beta$-stable (MoE $> 30$). In general, an MoE $\geq 10$ is needed to retain the $\beta$-phase in a metastable condition after cooling from the $\beta$-phase field.

$$\text{MoE} = 1.00\text{Mo} + 0.67\text{V} + 0.44\text{W} + 0.28\text{Nb} + 0.22\text{Ta} + 2.90\text{Fe}$$
$$+ 1.60\text{Cr} + 1.25\text{Ni} + 1.70\text{Mn} + 1.70\text{Co} - 1.00\text{Al}$$  

Data from this study can be found at Zenodo as a comma-separated-values (*.csv) file. The *.csv format is ubiquitous, and thus *.csv files can be easily imported into any software framework for further analysis. Moreover, the database can be easily updated using version control systems like git in this format.

Technical Validation

Outliers detection. Based on an in-depth analysis of key variables from the dataset (Fig. 1), we identified a dozen outliers, mainly regarding oxygen content and elongation. We double-checked these records and concluded that the oxygen contents in Xu et al. were indeed reported right; these specific studies are simply unusual, with relatively high oxygen additions. Entries with extreme elongation were associated with specimens that
did not fracture during mechanical testing; deformation at rupture values from these studies\textsuperscript{25,29–32} were set to a maximum of ±50%.

**Conflicting properties behavior.** A typical way of ranking structural materials is to observe strength-toughness relationships. Ideally, the material should present both features, but this rarely happens, as an increase in strength is often accompanied by a decrease in ductility\textsuperscript{33}. Here we offer a yield strength versus elongation at failure map to depict such a relationship for the materials compiled in the present dataset (Fig. 2). Limit lines clearly illustrate the expected behavior of conflicting properties. Low-alloy compositions (near-α, α + β) present a high strength with relatively low ductility.

On the other hand, near β and β-metastable alloys display a broad range of strength and elongations. The present dataset shows an extended range for these properties and more data points compared with recent reviews. It is also interesting to see how the dataset can be easily used for materials design.
Usage Notes
The dataset on Ti-based alloys is stored as a *.csv file that can be easily imported into any data analysis framework. Additionally, we provide a python script named utils.py (Python software foundation, version 3.8) with functions to filter the database, calculate the MoE parameter, and plot the figures from this article. We recommend the use of the pymatgen.Composition module to obtain pymatgen objects based on the formula for each data record. The use of pymatgen gives the user access to many other essential methods/functions inherited from pymatgen objects.

Code availability
The dataset and the utility script (utils.py) are available on Zenodo26, an open data repository. The python3 script is also available on GitLab (https://gitlab.com/comari/dax-ti), in which the users might obtain static (dax-ti-static) or a rolling release version (dax-ti-sid) of the project. The rolling release version will be continuously updated based on external requests. Researchers are encouraged to contribute to the database through GitLab or via e-mail, sharing their published data to expand the dataset.

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Competing interests
The authors declare no competing interests.

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