Supplementary Information Material for Mechanical performance dataset for alloy with applications at low temperatures

HaoxuanTang[1], Zhiyuan Chen[2], Xin Yao[2], and Zhiping Xu[*1]

[1]Applied Mechanics Laboratory, Department of Engineering Mechanics, Tsinghua University, Beijing, 100084, China.
[2]Beijing Minghui Tianhai Gas Storage and Transportation Equipment Sales Co., Ltd, Beijing 101100, China.
[*]Corresponding author(s). E-mail(s): xuzp@tsinghua.edu.cn

Supplementary Information

This Supplementary Information Material includes Supplementary Notes 1-3, Figures S1-3.

Supplementary Notes

1. The statistics of experimental data and the temperature dependence of mechanical properties of low-T alloys.
2. Strength–ductility–toughness synergy of low-T alloys at 77 K.
3. Hydrogen embrittlement behaviour of low-T alloys at 20 K.

Supplementary Figures

1. Temperature dependence of mechanical properties of low-T alloys.
2. Mechanical properties of low-T alloys at 77 K.
3. Hydrogen effects on the mechanical properties of low-T alloys.

Supplementary Note 1. The statistics of experimental data and the temperature dependence of mechanical properties of low-T alloys

The statistics of experimental data[1] are summarized in Fig. S1. The most explored alloys are the medium-entropy alloys (MEAs), steels, high-entropy alloys (HEAs), titanium, and aluminum alloys, which are sorted according to the strength-toughness data (Fig. S2). The remaining alloys are ranked by the number of reported data points. From the data contents, we find that steels with FCC structures, such as 300-series austenitic stainless steels (ASSs) containing Cr and Ni, are the most preferred material for low-temperature (low-T) applications due to their excellent low-T performance and mature production technology[2]. Al alloys feature the same face-centered cubic (FCC) structures as ASSs and display no significant ductile-to-brittle transition (DBT). It also has the advantage of low density and has been widely used in aerospace engineering. Ti alloys have high specific strengths, good corrosion resistance, and small coefficients of thermal expansion, and are relatively new in aerospace deployment. α- and β-Ti are hexagonal close-packed (HCP) and body-centered cubic (BCC), respectively. Most titanium alloys used in low-T applications are α-phase titanium alloys and two-phase titanium alloys containing a small amount of β-phase[3]. One of the latest developments of low-T alloys is the multi-principal element alloys (MPEAs), including MEAs and HEAs[4–7]. Composition engineering of MPEAs leads to excellent strength-toughness combinations for low-T applications. At low temperatures, specific compositions of MEA/HEA, such as CoCrFeNi with an FCC structure, exhibit nanotwinning in the later stages of deformation. The deformation mechanism dominated by twinning imparts ultra-high plasticity to these alloys. Additionally, the numerous low-energy interfaces generated by the twinning process effectively hinder dislocation movement, increase the work-hardening rate, and delay the onset of necking[8]. These developments and findings demonstrate the research activity of low-temperature alloys[9].

The relationships between the yield strength, tensile strength, fracture elongation, and temperature are plotted for MEAs, steels, HEAs, Ti and Al alloys (Fig. S1b-d). The mechanical properties are compared at temperatures from 4.2 K, 20 K, 77 K, 110 K, to room temperature (RT). Ti alloys show the highest yield strengths at low temperature, followed by MEAs, HEAs, and steels with similar yield strengths. The strengths of Al alloys are the lowest (Fig. S1b). MEAs, HEAs, steels, and Ti alloys show similar tensile strengths at low temperature, followed by Al alloys (Fig. S1c). As the temperature decreases, the overall tensile strengths increase in general. MEAs and HEAs demonstrate exceptional low-T ductility, with fracture elongation ($\sim 60\%$) much higher than that of steels ($\sim 40\%$). Ti alloys exhibit the poorest ductility at low temperature due to their HCP structures (Fig. S1d).

Supplementary Note 2. Strength–ductility–toughness synergy of low-T alloys at 77 K

The low-T data are relatively rich above 77 K but rare in the ranges of $0 - 4.2$ K, $4.2 - 20$ K, and $20 - 77$ K. The reason is that liquid nitrogen refrigeration (> 77 K) is much more cost-effective than the liquid helium technology ($4.2 - 77$ K). There are very few experiments (12/1253) using LH2 refrigeration where the effect of hydrogen embrittlement can be explored, mainly due to safety concerns. Interestingly, there is a gap between 20 and 77 K, where the physics behind the mechanical performance of low-T alloys remains unclear.

Data analysis is first conducted for the data points at 77 K (Fig. S2). The ratio R between the yield and tensile strengths is calculated to measure the strength reserve of materials. As the yield strength approaches the tensile strength, there is either a very short or no yield, and brittle fracture is expected. A low value of R suggests low strength utilization. The R values of Al and Ti alloys are close to 1, indicating their brittleness. Data dispersion for MPEAs and steels is diverse but suggests better plasticity at low temperature. Data in Fig. S2 shows that MPEAs and steels exhibit a significant overlap in both the strength-ductility and strength-toughness diagrams, but MPEAs are superior to steels in balancing the trade-offs.

Supplementary Note 3. Hydrogen embrittlement behaviour of low-T alloys at 20 K

The material performance at the LH2 condition is chosen here as a specific example for discussion. The world is heading for hydrogen, and a large-scale hydrogen economy is essential for a clean energy future[10]. LH2 storage and transportation are promising solutions for large-scale and long-distance applications. The mechanical performance of 300-series ASSs under LH2/hydrogen charging (HC) conditions at 20 K is compared with that in helium conditions (Fig. S3). The results show that the effect of LH2 and hydrogen filling conditions (*e.g.*, electrochemical hydrogen charging) on the strength and fracture elongation is not significant. However, the reduction of area (RA) decreases significantly compared with the helium cooling condition, signaling the hydrogen embrittlement effect[11]. Another study shows that the RA at $80 - 100$ K hydrogen remains the same as that in a liquid nitrogen environment, and thus no hydrogen embrittlement[12]. Possible reasons for the observed contradiction include a potential new hydrogen embrittlement mechanism occurring between 20-80 K and the varying susceptibility of alloys to hydrogen embrittlement in different environments, such as gaseous hydrogen, LH2, and electrochemical hydrogen charging.

Supplementary Figures and Figure Captions

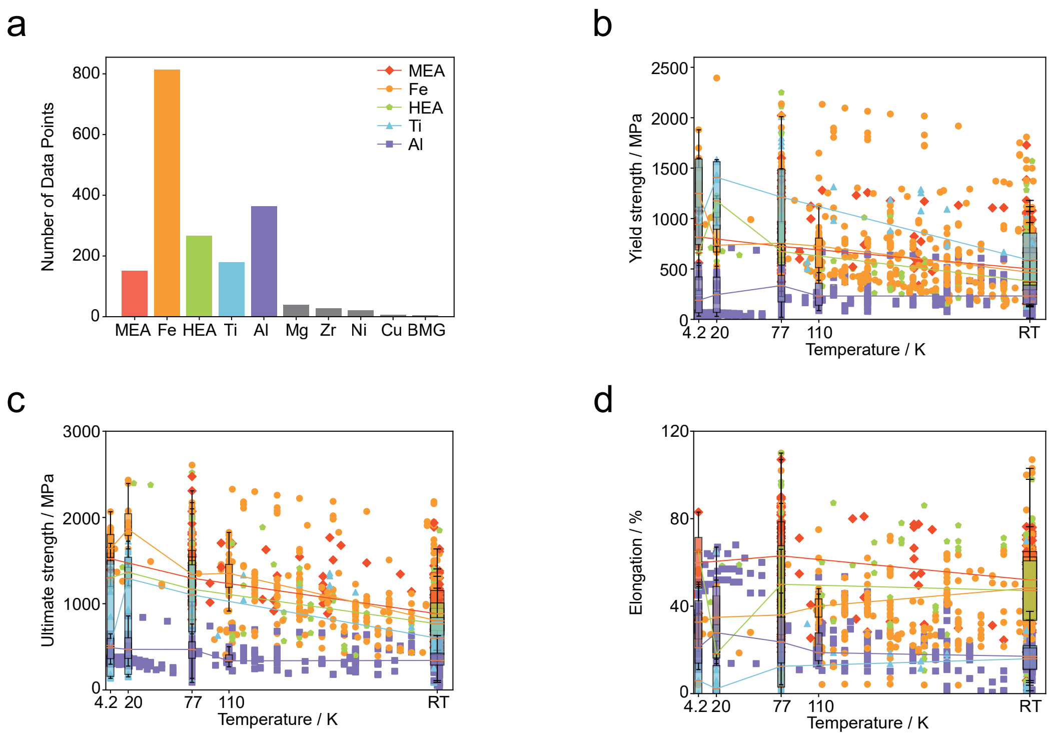

Figure S1: Temperature dependence of mechanical properties of low-T alloys[1]. (a) Histogram of the number of data points for each alloy. Representative (b) yield strength-temperature (σ_{y}-T), (c) ultimate tensile strength (σ_{u}-T), and (d) elongation-temperature (e-T) data of low-T alloys. Box plots are added at representative temperatures (4.2 K, 20 K, 77 K, 110 K, RT).

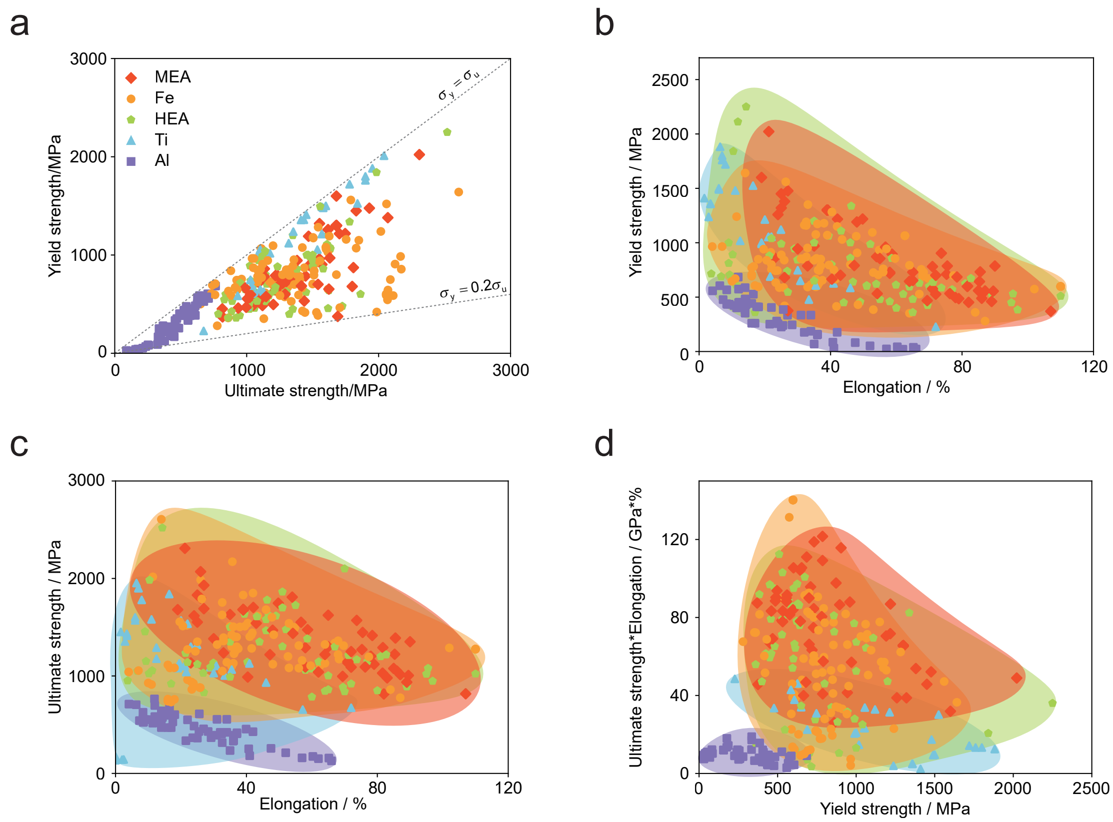

Figure S2: Mechanical properties of low-T alloys at 77 K[1]. (a) Relation between yield strength σ_y, and UTS, σ_u at 77 K. References $\sigma_\mathrm{y} = \sigma_\mathrm{u}$ and $\sigma_\mathrm{y} = 0.2\sigma_\mathrm{u}$ are added as the dashed lines. (b-d) Ashby maps in terms of (b) the yield strength versus fracture elongation, (c) the ultimate strength versus fracture elongation, and (d) the product of ultimate strength and fracture elongation versus the yield strength at 77 K. Strength-ductility and strength-toughness relationships at 77 K.

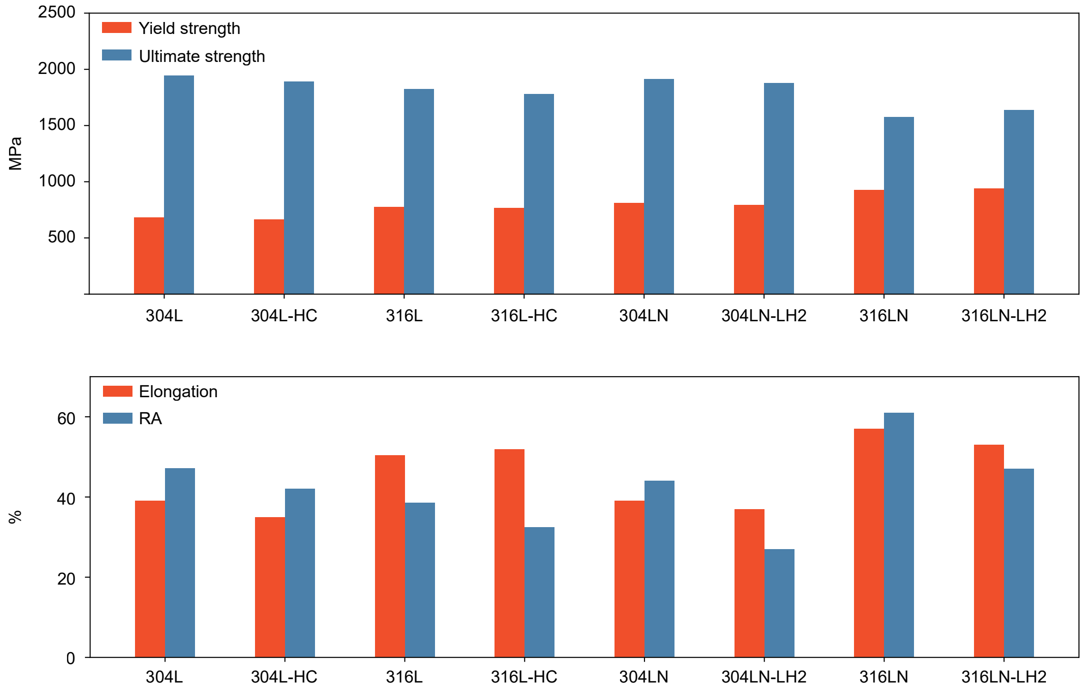

Figure S3: Hydrogen effects on the mechanical properties of low-T alloys[1, 13]. Mechanical properties of selected 300-series austenitic stainless steels (ASSs) at 20 K in helium gas, liquid hydrogen (LH2), and hydrogen-charged (HC) conditions.

References

[1] Tang, H. & Xu, Z. Mechanical performance dataset for alloy with applications at low temperatures. *figshare*. https://doi.org/10.6084/m9.figshare.25912267 (2024).

[2] Qiu, Y., Yang, H., Tong, L. & Wang, L. Research progress of cryogenic materials for storage and transportation of liquid hydrogen. *Metals* **11**, 1101 (2021).

[3] Zang, M. *et al.* Cryogenic tensile properties and deformation behavior of a fine-grained near alpha titanium alloy with an equiaxed microstructure. *Mater. Sci. Eng. A* **840**, 142952 (2022).

[4] Zhang, D., Zhang, J., Kuang, J., Liu, G. & Sun, J. Superior strength-ductility synergy and strain hardenability of Al/Ta co-doped NiCoCr twinned medium entropy alloy for cryogenic applications. *Acta Mater.* **220**, 117288 (2021).

[5] Bian, B. *et al.* A novel cobalt-free FeMnCrNi medium-entropy alloy with exceptional yield strength and ductility at cryogenic temperature. *J. Alloys Compd.* **827**, 153981 (2020).

[6] Tong, Y. *et al.* Outstanding tensile properties of a precipitation-strengthened $FeCoNiCrTi_{0.2}$ high-entropy alloy at room and cryogenic temperatures. *Acta Mater.* **165**, 228–240 (2019).

[7] Liu, D. *et al.* Exceptional fracture toughness of CrCoNi-based medium-and high-entropy alloys at 20 Kelvin. *Science* **378**, 978–983 (2022).

[8] Otto, F. *et al.* The influences of temperature and microstructure on the tensile properties of a cocrfemnni high-entropy alloy. *Acta Materialia* **61**, 5743–5755 (2013).

[9] Wang, F. *et al.* Shearing brittle intermetallics enhances cryogenic strength and ductility of steels. *Science* **384**, 1017–1022 (2024).

[10] Aziz, M. Liquid hydrogen: A review on liquefaction, storage, transportation, and safety. *Energies* **14**, 5917 (2021).

[11] Deimel, P. & Sattler, E. Austenitic steels of different composition in liquid and gaseous hydrogen. *Corros. Sci.* **50**, 1598–1607 (2008).

[12] Fukuyama, S., Sun, D., Zhang, L., Wen, M. & Yokogawa, K. Effect of temperature on hydrogen environment embrittlement of type 316 series austenitic stainless steels at low temperatures. *J. Jpn. Inst. Met.* **67**, 456–459 (2003).

[13] Xu, Z. in *Comprehensive Structural Integrity (Second Edition)* (eds Aliabadi, M. H. F. & Soboyejo, W. O.) second edition edn. (Elsevier, Oxford, 2023), pp. 131-162.