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On the yield stress anomaly in a B2-ordered refractory $AlNbTiVZr_{0.25}$ high-entropy alloy

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A B S T R A C T

High-entropy intermetallics have a great potential for high-temperature applications. However, there is relatively limited information about the plastic flow behaviour and deformation mechanisms of these materials. Here we reported a yield strength anomaly (YSA) in a refractory $AlNbTiVZr_{0.25}$ high-entropy alloy with a multicomponent B2 matrix phase. The YSA was detected during the compression tests at 22–900 °C with a stress peak at 700 °C. Detailed analysis suggested that the YSA could be connected with the glide of dissociated $a\langle 111\rangle$ superdislocations.

1. Introduction

Due to excellent specific strength and oxidation resistance at elevated temperatures, intermetallics have been considered substitutes for existing high-temperature materials in gas turbine engines for the last 50 years [1]. However, notorious brittleness and scattered properties hamper their wide application as structural materials [2].

Among numerous strategies, alloying seems one of the most suitable and effective approaches for harmonising the performance of intermetallics [3]. The recently introduced high-entropy alloys (HEAs) concept offers a new avenue in tuning the properties of intermetallics and their formation in unexpected systems [4–7]. Specifically, Al-containing B2 phases are absent in binary Al-ETM (ETM-early transition metal) systems but become stable in refractory high-entropy alloys (RHEAs), which are deemed as new potential high-temperature materials [8,9].

Although many studies are devoted to the microstructure design of B2-RHEAs [10,11], plastic flow behaviour and deformation mechanisms of multicomponent B2 phases remain less explored [11–13]. Of different features, a yield stress anomaly (YSA) attracts great attention. The YSA is a positive temperature dependence of strength, typical for some materials, including binary and ternary B2 compounds [13–16]. This work discussed the YSA manifestation in a B2-matrix $AlNbTiVZr_{0.25}$ RHEA [17,18] in a temperature interval of 600–800 °C. The reasons responsible for the YSA were carefully addressed.

2. Materials and methods

Details of the manufacturing and heat treatment procedures of the alloy are presented elsewhere [17,18]. The phase composition and microstructure of the alloy were studied using scanning and transmission electron microscopes (SEM and TEM) equipped with energy-dispersive (EDS) detectors. Data on the actual chemical composition of the alloy are given in Table S1 (Supplementary Material).

Compression tests were performed using rectangular specimens measured $5 \times 3 \times 3$ mm^3 at 22–900 °C and the initial strain rate of 10^{-4} s^{-1}. Three specimens were tested at each temperature to ensure data reproducibility. Additional compression tests were conducted at 700 °C and the initial strain rates of 10^{-4}, 5×10^{-4}, 10^{-3}, 5×10^{-3} s^{-1}, which were then interrupted at $\varepsilon \approx 1\%$. To arrest the structure after compression, the samples were quenched in water immediately after the test termination. Dislocation analysis was conducted for the specimens compressed at 700 °C and 10^{-4} s^{-1} applying two-beam Bragg-contrast imaging. Burgers vectors, $\vec{b}$, of dislocations were identified using the $\vec{g} \times \vec{b} = 0$ criterion for dislocation invisibility.

3. Results and discussion

Detailed analysis of the microstructure of the $AlNbTiVZr_{0.25}$ alloy is given elsewhere [17,18]. Here, only a brief of information is presented. The studied alloy consisted of a multicomponent B2 (*CsCl-prototype; cP2;*

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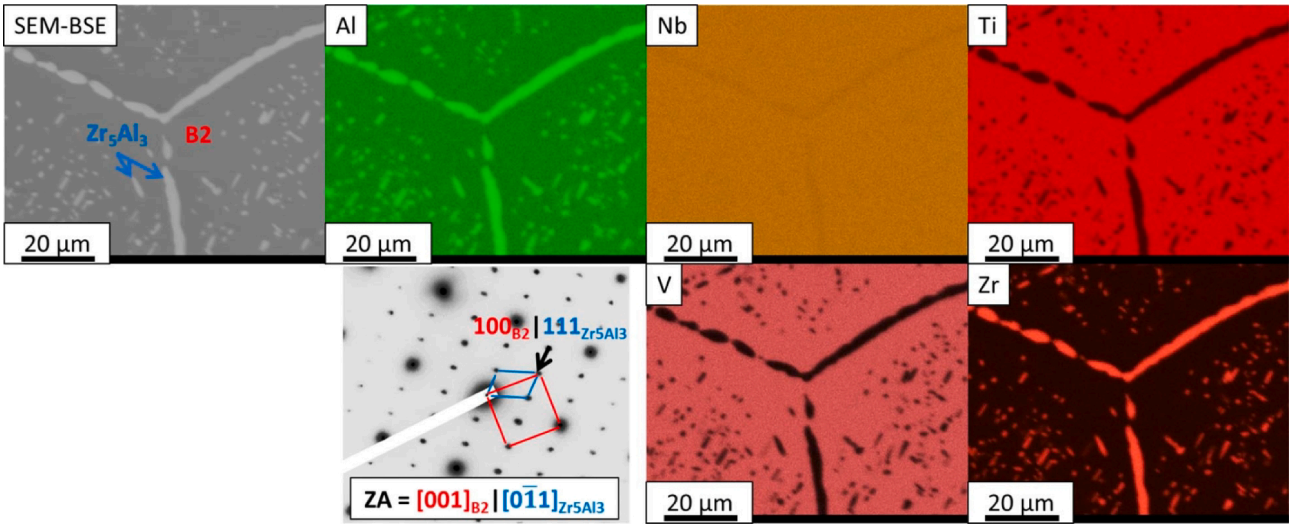

Fig. 1. A typical microstructure of the $AlNbTiVZr_{0.25}$ alloy: SEM-BSE image, SEM-EDS maps, and SAED pattern showing the B2 matrix and Zr_5Al_3 precipitates with the $(1\,0\,0)_{B2}||(1\,1\,1)_{Zr5Al3}$, $[0\,0\,1]_{B2}||[0\ \bar{1}\ 1]_{Zr5Al3}$ OR.

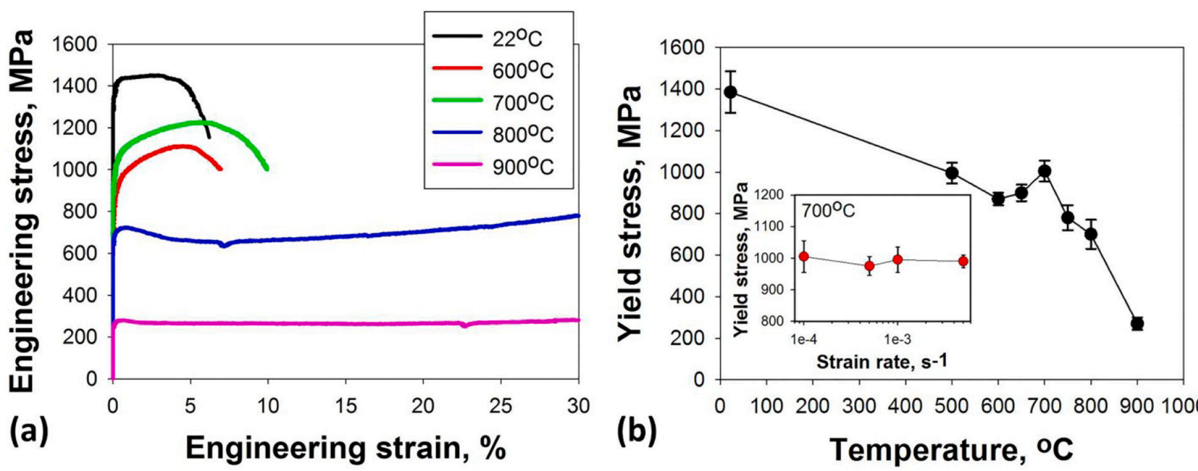

Fig. 2. Mechanical properties evaluation of the $AlNbTiVZr_{0.25}$ alloy: (a) – engineering stress – engineering strain curves obtained during compression tests at 22–900 °C; (b) – temperature and strain rate (for 700 °C) dependence of the yield stress.

Pm-3m) matrix and (Zr, Al)-rich precipitates (identified as Zr_5Al_3-type phase (*Mn_5Si_3-prototype; hP16; $P6_3/mcm$*)) with a volume fraction of ~ 10% and a specific orientation relationship (Fig. 1; Fig. S1, Supplementary Material).

The alloy showed limited ductility ($\varepsilon < 10\%$) at 22–700 °C and weak (22 °C) or notable (500–700 °C) strain hardening before fracturing (Fig. 2(a); Fig. S2 and Table S2, Supplementary Material). At 750–900 °C, short strain hardening and softening, and prolonged steady-state flow stages, resulting in ductility increment, were observed (Fig. 2 (a); Fig. S2, Supplementary Material). However, the temperature dependence of the yield stress, YS, was more intriguing (Fig. 2(b)). The alloy demonstrated high YS (1385 MPa) at 22 °C, which gradually decreased when the testing temperature increased to 600 °C (870 MPa). Then the YS raised between 600 and 700 °C, reaching a stress peak at 700 °C (1005 MPa), and dropped again at T > 700 °C (Fig. 2(b); Fig. S2 and Table S2, Supplementary Material). Notably, the YS at 700 °C was insensitive to strain rate variations (insert in Fig. 2(b)).

Similar positive temperature dependence of the YS, called a yield stress anomaly (YSA), was previously found in binary and ternary B2 compounds [13–16]. However, there are scarce data on this phenomenon in the B2-ordered (R)HEAs. For example, the YSA was recently reported for an $Al_{10}Nb_{15}Ta_5Ti_{30}Zr_{40}$ RHEA composed of a nanoscale mixture of bcc and B2 phases [19]. In that case, the YSA was attributed to the phase decomposition. Meanwhile, such an explanation is invalid for the studied alloy since its structure was relatively stable after compression at the stress peak temperature (700°C); yet, some coagulation/aggregation of the Zr_5Al_3 particles should be noted (Fig. 3(a)).

To gain insight into the origins of the YSA in the $AlNbTiVZr_{0.25}$ alloy, we conducted a detailed TEM study (Fig. 3(b–f)). Post-mortem microstructure observation in a dark-field mode showed the presence of multiple dissociated dislocations in the B2 matrix (Fig. 3(b)), morphologically similar to those observed in binary B2 compounds [20,21]. Decomposed $a\ \langle 1\,1\,1\rangle$ superdislocations comprising two $\frac{a}{2}\ \langle 1\,1\,1\rangle$ partial dislocations linked by an antiphase boundary (APB) are usual in such intermetallics [22]. For the $AlNbTiVZr_{0.25}$ alloy, imaging under different diffraction conditions ($\vec{g}$) discovered that all the dislocations stayed visible for $\vec{g} = 110$, 200, and $0\ \bar{2}\ 0$, but became completely invisible when $\vec{g} = 1\ \bar{1}\ 0$ (Fig. 3(c–f)). This $\vec{g} \times \vec{b} = 0$ analysis testifies that plastic deformation in the studied alloy at 700 °C was governed by the glide of paired $\frac{a}{2}\ \langle 1\,1\,1\rangle$ partial dislocations (or dissociated $a\langle 1\,1\,1\rangle$ superdislocations).

The dissociation width of superdislocations in ordered alloys affects their mechanical properties [16,23,24] and depends on an APB energy

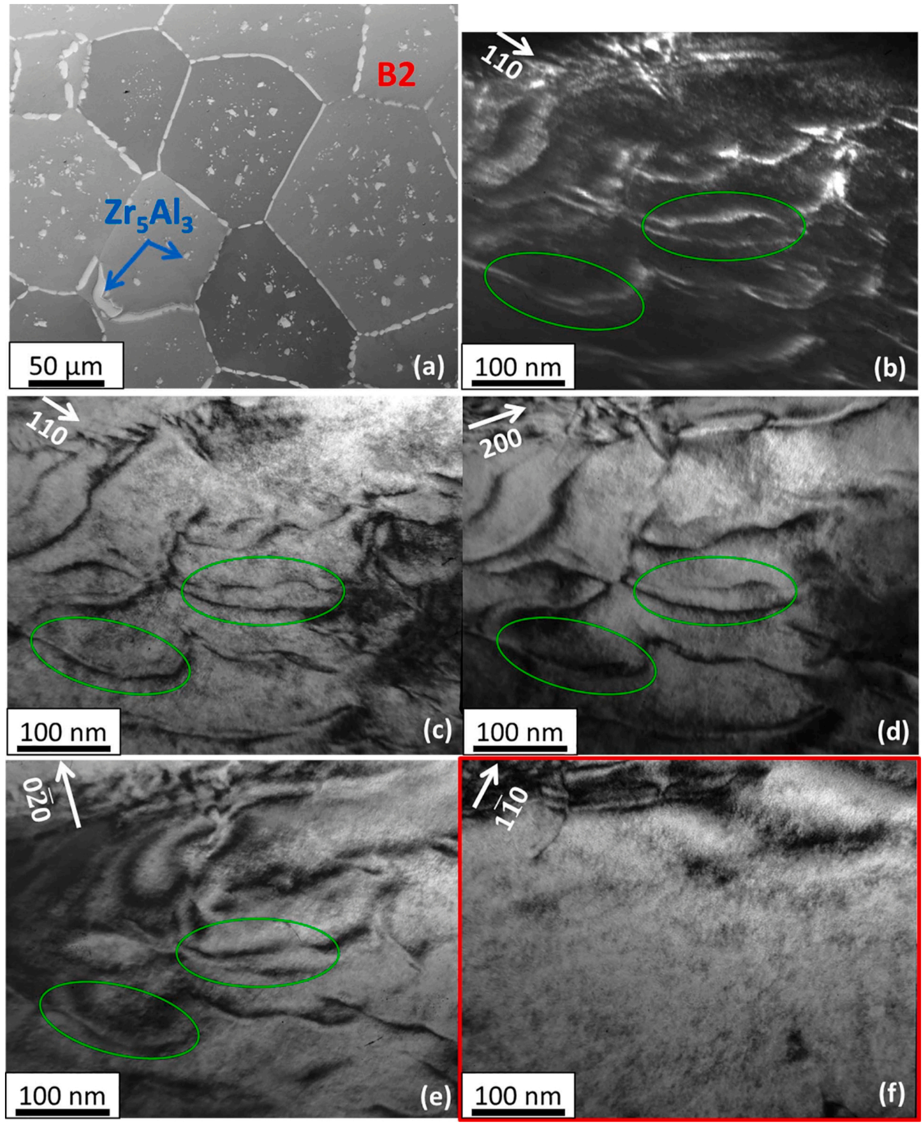

Fig. 3. Microstructure investigations of the $AlNbTiVZr_{0.25}$ alloy compressed at 700 °C to $\varepsilon \approx 1\%$: (a) – SEM-BSE image (the compression axis is vertical); (b) – TEM dark-field image taken under a two-beam condition with $\vec{g} = 110$ near the [001] zone axis showing typical dislocation structure of the B2 matrix; (c–f) – TEM bright-field images taken under a two-beam condition with $\vec{g} = 110$ (c), 200 (d), $0\ \bar{2}\ 0$ (e), and $1\ \bar{1}\ 0$ (f).

[16,20,23,24]. Marcinkowski and Miller [23] connected an increased spacing (or reduced APB energy) between two partials in a Ni_3Mn compound with a decreased degree of long-range order, S. In turn, Crawford and Ray [20] showed a strong dependence of the APB energy on the chemical composition: the dissociation width lowered in B2/$D0_3$ Fe-Al alloys when the Al content rose from 26 to 36 at.%. Based on these works, two different interpretations of the YSA were given later [16,25] (see for details Supplementary Material).

Specifically, the framework by Marcinkowski and Miller [23] laid the foundation of a well-accepted order–disorder strengthening mechanism by Stoloff and Davies [16]. They suggested that, at intermediate S, $\frac{a}{2}\langle 111\rangle$ partial dislocations of dissociated $a\ \langle 111\rangle$ superdislocations in a B2 FeCo-2 V alloy could move independently, leaving APB trails, and, thus, contributed to strength greatly than undissociated $a\ \langle 111\rangle$ superdislocations at high S or unit $\frac{a}{2}\ \langle 111\rangle$ dislocations at low S. Recently, Liao and Baker [24] also showed that thermal-induced decreasing of S reduced the APB energy in an $L2_1$ Fe_2MnAl compound, thereby leading to a decoupling of $\frac{a}{2}\ \langle 111\rangle$ partial dislocations. The glide of these partial dislocations produced APB ribbons in the matrix, resulting in the stress peak at 427–527 °C.

According to Stoloff and Davies [16], the spacing between two $\frac{a}{2}$ $\langle 111\rangle$ partials of decomposed $a\ \langle 111\rangle$ superdislocations that induced the YSA was $r \approx 15$ nm. This distance correlates well with the dissociation width ($r \approx 10$ nm) observed in the $AlNbTiVZr_{0.25}$ alloy at 700 °C (Fig. 3(a–e)). Considering the above data, the motion of dissociated a $\langle 111\rangle$ superdislocations can be inferred as the most probable reason for the YSA in the studied alloy. An indirect indication for the operation of this mechanism is the strain rate insensitivity at 700 °C (insert in Fig. 2 (b)) [24].

In the broader context, the current study results endow opportunities to balance the properties of B2-ordered RHEAs. By adjusting the dissociation width of superdislocations through controlling of S [17], we can design new multicomponent intermetallics with room-temperature tensile ductility and promising high-temperature strength. However, additional experimental work is required to verify this suggestion.

4. Conclusions

Here we investigated the mechanical properties of the $AlNbTiVZr_{0.25}$ RHEA with the multicomponent B2 matrix during compression tests at

22–900 °C. The alloy showed conventional (negative) temperature dependence of the YS at 22–600 °C and 800–900 °C. At 600–800 °C, we observed the YSA with the stress peak at 700 °C. Detailed TEM investigations revealed that the motion of dissociated $a\langle 111\rangle$ superdislocations mediated the plastic deformation at 700 °C. Such dislocations were assumed to invoke the YSA.

CRediT authorship contribution statement

N. Yurchenko: Conceptualization, Methodology, Investigation, Validation, Visualization, Writing – original draft, Writing – review & editing, Supervision, Project administration, Funding acquisition. **E. Panina:** Investigation, Validation. **A. Belyakov:** Validation, Writing – review & editing. **G. Salishchev:** Writing – review & editing. **S. Zherebtsov:** Writing – review & editing. **N. Stepanov:** Supervision, Writing – review & editing.

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.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.matlet.2021.131584.

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