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1 Deformation mechanisms in hexagonal 2 close-packed high-entropy alloys

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14 ABSTRACT

15 Single-phase hexagonal close-packed structure of the ScYLaGdTbDyHoErLu high-entropy alloy was studied in detail. The applicability of the
16 rule of mixture was analyzed with respect to the lattice constant, mechanical parameters, elastic properties, melting point, and hardness of the
17 alloy. Significant tension-compression asymmetry has been found and explained by the strength differential effect during the uniaxial tests.
18 Numerous deformation twins and high densities of stacking faults can be observed from the morphological characterization by a transmission
19 electron microscope, which governs the main deformation mechanism during the plastic deformation in the current **high-entropy alloys**.

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21 I. INTRODUCTION

22 High-entropy alloys (HEAs) that are mainly defined from the
23 viewpoint of composition and configuration entropy have attracted
24 widespread attention in the materials community from 2004.¹⁻³
25 One is that the alloys contain five or more principal elements in an
26 equimolar or near-equimolar ratio, and each element accounts for
27 5%–35% [atomic percent (at. %)]. The other is that the alloys have
28 a value of the configuration entropy at least $1.5R$ in a random
29 chaos system (R is the gas constant). As soon as they appeared,
30 researchers have given them much attention because of their
31 unique properties, including high hardness and strength,⁴ unique
32 corrosion resistance,^{5,6} high thermal stability,^{7,8} excellent irradiation
33 resistance,^{9,10} good magnetic properties,^{11,12} and outstanding frac-
34 ture, fatigue, and thermoelectric properties.¹³⁻¹⁵

35 It is attractive that some single-phase HEAs that are thermo-
36 dynamically metastable can be prepared by mixing multi-principal
37 elements. At present, representative HEAs possess exact near-
38 equimolar ratios, including body-centered-cubic (BCC) TiZrHfNbTa
39 HEA¹⁶ and face-centered-cubic (FCC) CoCrFeMnNi HEA.¹⁷ In con-
40 trast, hexagonal close-packed (HCP) HEAs were rarely reported.^{18,19}

41 The HEAs with HCP structures mainly consisted of rare-earth ele-
42 ments, which presented similar atomic sizes and crystal structures.

43 The HCP HEAs were synthesized by arc-melting taking the com-
44 positions of YGdTbDyLu,²⁰ GdTbDyTmLu,²⁰ HoDyYGdTb,²¹⁻²⁴

GdHoLaTbY,¹⁸ ScYLaTiZrHf,²⁵ GdHoErTbDy,²⁶ CeGdTbDyHo,²⁷ 45
Ir₂₆Mo₂₀Rh_{22.5}Ru₂₀W_{11.5},²⁸ Ir_{22.5}Mo₂₀Rh₂₀Ru₂₅W_{9.5},²⁸ AlHfScTiZr,²⁹ 46
Tb_{20.3}Dy_{20.7}Ho_{20.3}Er_{19.7}Tm₁₉,³⁰ and ScTiZrHf.³¹ A novel preparation 47
method, the thermal decomposition of single-source precursors, was 48
adopted for the fabrication of IrOsReRhRu HCP HEA.³² 49

50 Overall, most developed HCP HEAs were composed of 50
rare-earth elements, and only a few studies focused on the mechan- 51
ical behavior, not as thoroughly investigated as in BCC and FCC 52
HEAs. Recently, Qiao *et al.* investigated the strengthening behavior 53
in DyErGdHoLuScTbY, DyGdHoLaTbY, and ErGdHoLaTbY HCP 54
HEAs and found that the solid-solution strengthening (SSS) was 55
weak in rare-earth HCP HEAs compared with that in BCC and 56
FCC HEAs.^{18,19} The deformation mechanisms were still not under- 57
stood clearly up to now. Therefore, one goal of this research is to 58
explore the limit of the number of principal components in 59
rare-earth based HCP HEAs. Moreover, another objective is to 60
investigate the mechanical properties and deformation mechanisms 61
of the newly designed rare-earth based HCP HEA. 62

63 II. RULES OF HCP STRUCTURE HEAS

64 The phase formation is mainly predicted by the phase 64
diagram for traditional alloys, but the phase diagrams of HEAs 65
with more constituent elements are not available. Hence, several 66
criteria, including the enthalpy of mixing (ΔH_{mix}), entropy of 67

68 mixing (ΔS_{mix}), atomic-size difference (δ),³³ valence electron con-
69 centration (VEC), and ϕ -parameter based on thermodynamics,
70 were proposed to predict the phase formation in various HEAs.
71 The configurational entropy, ΔS_{conf} , can be obtained by

$$\Delta S_{conf} = R \ln N, \quad (1)$$

72 where R is the gas constant and N is the number of elements.
73 Mixing the constituent elements with an equiatomic ratio, ΔS_{mix}
74 can reach the maximum value based on Eq. (1). The stability of
75 HEAs is determined by ΔH_{mix} and ΔS_{mix} together.¹⁷ δ and ΔH_{mix}
76 are defined as follows:

$$\delta = \sqrt{\sum_{i=1}^N c_i (1 - r_i/\bar{r})^2}, \quad (2)$$

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$$\Delta H_{mix} = 4 \sum_{i=1, i \neq j}^n \Delta H_{ij} c_i c_j, \quad (3)$$

where c_i (and c_j) is the atomic fraction of the i th (and j th) compo-
nent, r_i is the atomic radius of the i th constituent element, and
 $\bar{r} (= \sum c_i r_i)$ is the average atomic radius of the alloy, ΔH_{ij} is the
mixing¹ enthalpy of a binary liquid alloy, which can be acquired
from the empirical model in the liquid state.³⁴ In addition, Yao
et al. found that it is preferent for HEAs to form solid solution if
the atomic-size difference (δ) is lower than 5.5.³⁵ Recent studies
indicated that HEAs show the single-phase solid solution structures
when $-16.25 \text{ kJ/mol} \leq \Delta H_{ij} \leq \pm 5 \text{ kJ/mol}$.³⁶
The single ϕ -parameter is defined as³⁷

$$\phi = \frac{\Delta S_{mix} - |\Delta H_{mix}|/T_m}{|S_E|}, \quad (4)$$

88 where S_E is the excessive entropy of mixing, which is modeled as a
89 function of atomic size and atomic packing. T_m is the melting
90 point of the alloy. It is found that the single-phase solid solutions
91 are generally formed for multicomponent HEAs with $\phi > \phi_c$, and

amorphous phases or multiphases with $\phi < \phi_c$. Gao *et al.* identi-
fied the criteria ϕ_c with the value of 7.³⁶ The basis for the forma-
tion of a single-phase HEA can be described by these critical
parameters (ΔH_{mix} , ΔS_{mix} , δ , and ϕ). Besides, VEC can be used to
judge the phase formation,

$$VEC = \sum_{i=1}^n c_i (VEC)_i, \quad (5)$$

where $(VEC)_i$ is the VEC of the i th element. It is currently believed
that the present HEAs possess the HCP structure with $VEC \cong 3$.³⁷⁻³⁹
These parameters of different single HCP HEAs together with the
ScYLaGdTbDyHoErLu alloy are summarized in Table I. Therefore, it
can be inferred that the ScYLaGdTbDyHoErLu alloy can form a
single-phase HCP HEA based on these parameters.

III. EXPERIMENTAL PROCEDURES

Equiatomic ScYLaGdTbDyHoErLu ingots were prepared
by vacuum arc melting in the Ti-gettered high-purity argon
atmosphere using high-purity elements (weight purity $\geq 99.9\%$).
The ingots were remelted six times to ensure the chemical homoge-
neity. The structures of the alloys were characterized by x-ray
diffraction (XRD) using the Cu $K\alpha$ radiation in the 2θ range of
 20° – 80° . Optical microscopy (OM) and scanning electron micros-
copy (SEM) were employed to observe the microstructures of the
alloys, and an energy dispersive spectrometer (EDS) was used to
analyze chemical compositions. The structures of as-cast and
deformed alloys were further analyzed by the JEM-F200 transmis-
sion electron microscopy (TEM), selected area electron diffraction
(SAED), and high-resolution transmission electron microscopy
(HRTEM). The TEM samples were prepared by ion-beam thinning.
Elastic properties of the alloys were investigated by resonant ultra-
sound spectroscopy (RUS) with the rod-like samples under a gauge
dimension of $\phi 3 \times 2.5 \text{ mm}$. The thermal properties of the alloys
were examined by a differential scanning calorimetry (DSC) at a
rate of 15 K/min from room temperature (298 K) to 1773 K under a
high purity argon atmosphere.

TABLE I. The different thermodynamic parameters of the single HCP HEAs. R is the gas constant, $R = 8.314 \text{ J mol}^{-1} \text{ K}^{-1}$.

Alloys	S_{conf} ($\text{J mol}^{-1} \text{ K}^{-1}$)	ΔH_{mix} (kJ mol^{-1})	Δ (%)	VEC	ϕ	Reference
ScYLaGdTbDyHoErLu	2.20R	0.4	3.4	3	55.1	This work
GdHoLaTbY	1.51R	0	2.2	3	97.5	18
DyGdHoLaTbY	1.79R	0	2.1	3	116.2	19
ErGdHoLaTbY	1.79R	0.1	2.2	3	100.8	19
DyErGdHoLuScTbY	2.1R	0.3	2.8	3	79.1	19
YGdTbDyLu	1.61R	0	1.6	3	245.9	20
GdTbDyTmLu	1.61R	0	1.4	3	18.8	20
HoDyYGdTb	1.61R	0	0.8	3	701.5	21
GdDyErHoTb	1.61R	0	0.9	3	626.6	26
$\text{Al}_{15}\text{Hf}_{25}\text{Sc}_{10}\text{Ti}_{25}\text{Zr}_{25}$	1.55R	-17.5	4.9	3.75	5.8	29
$\text{Tb}_{20.3}\text{Dy}_{20.7}\text{Ho}_{20.3}\text{Er}_{19.7}\text{Tm}_{19}$	1.61R	0	4.8	3	21.3	30
ScTiZrHf	1.38R	4.3	4.3	3.75	18.5	31

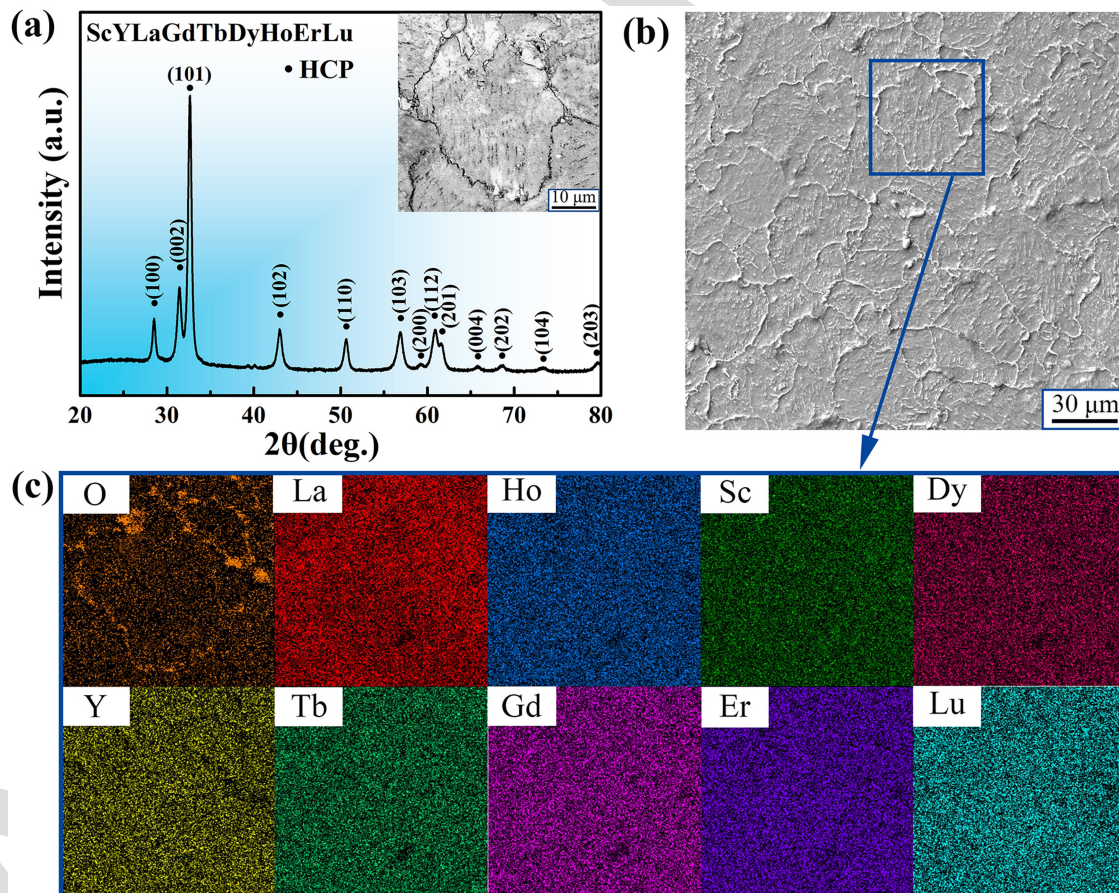
124 The Vickers hardness tests were conducted by a load of 200 g
 125 with a dwell time of 15 s. Each sample was measured 12 times, and
 126 the average value was taken to ensure the consistency. The tensile
 127 samples were cut from the ingots, which were dog-bone-like shape
 128 with a gauge dimension of 10 mm in length, 3 mm in width, and
 129 2 mm thick. The compressive testing specimens with a diameter of
 130 3 mm and a height of 6 mm were cut from the ingots by a wire-
 131 electrode cutting machine. All the surfaces were grinded and the
 132 two end's surface were carefully polished to guarantee acceptable
 133 parallelism with an aspect ratio (height/diameter) of 2:1 to an accu-
 134 racy of $5\ \mu\text{m}$. It should be pointed out that these samples were not
 135 rolled because of the formation of cracks, although the deformation
 136 in each pass during the rolling was very low. The strain rates of
 137 compression and tension tests were $5 \times 10^{-4}\ \text{s}^{-1}$ and carried out by
 138 an Instron 5969 mechanical testing machine. One strain gauge with
 139 the size of $9 \times 3\ \text{mm}$ was pasted on the gauge section of the sample
 140 to measure the strain during each tension test. Both the compres-
 141 sion and tension tests were done at least three times to make sure
 142 the accuracy and repeatability of the results.

143 IV. RESULTS

144 A. Microstructures

145 Figure 1(a) shows XRD patterns of the as-cast 145
 ScYLaGdTbDyHoErLu alloy. It is obvious that only a set of the 146
 HCP structure existed, in agreement with the theoretical prediction, 147
 which will be discussed in detail in Sec. V. The lattice parameter of 148
 the alloy was determined to be $a = 0.36\ \text{nm}$, $c = 0.5655\ \text{nm}$, and 149
 $c/a = 1.5708$. The lattice constants of the alloy and its constituent 150
 elements are summarized in Table II. The OM pictures indicated 151
 equiaxial grains in the present ScYLaGdTbDyHoErLu alloy, as 152
 shown in the inset of Fig. 1(a). 153

154 The average grain size of the ScYLaGdTbDyHoErLu alloy that 154
 measured and calculated by OM was $38\ \mu\text{m}$, which is in accordance 155
 with the SEM result, as presented in Fig. 1(b). Employing EDS 156
 mapping for a blue-colored rectangular area from Fig. 1(c), it is 157
 apparent that the elements distributed uniformly within the grains. 158
 The significant differences cannot be detected within the experimen- 159
 tal uncertainty ($\text{Sc}_{11.1}\text{Y}_{11.4}\text{La}_{11.8}\text{Gd}_{11.8}\text{Tb}_{10.6}\text{Dy}_{10.7}\text{Ho}_{10.5}\text{Er}_{11.4}\text{Lu}_{10.7}$ 160



161 **FIG. 1.** (a) XRD pattern of the as-cast ScYLaGdTbDyHoErLu HEA. The inset in (a) is the OM image of the current alloy. (b) and (c) show the SEM micrograph and EDS mapping, respectively.

TABLE II. Lattice constants, a , c , and c/a ratios of the ScYLaGdTbDyHoErLu HEA, and single constituent elements. The calculated values are obtained by the RoM.

Alloy and elements		a (nm)	c (nm)	c/a
ScYLaGdTbDyHoErLu	Exp. cal.	0.360 0	0.565 5	1.5708
		0.357 8	0.566 2	1.5826
Sc	...	0.330 9	0.527 3	1.5935
Y	...	0.364 74	0.573 06	1.5711
La	...	0.377 2	0.607 2	1.6098
Gd	...	0.363 6	0.578 26	1.5904
Tb	...	0.360 1	0.569 36	1.5811
Dy	...	0.359 3	0.565 37	1.5735
Ho	...	0.357 73	0.561 58	1.5698
Er	...	0.355 88	0.558 74	1.5700
Lu	...	0.350 31	0.555 09	1.5846

161 similar to the normal composition). Moreover, a strong fluctuation
162 of the elemental distribution was observed at the grain boundary.
163 Each rare-earth element distributed inside the grains homogeneously
164 (~ 6.9 at. % for each other elements), and some oxygen appeared at
165 the grain boundary. The similar distribution has been reported in
166 previous studies on rare-earth HCP HEAs with precipitates, and the
167 element of oxygen was enriched at grain boundaries as well.^{18,19,40}
168 The oxygen was mainly from the raw material due to the exposure
169 during the fabrication and/or transportation of the material, since
170 rare-earth metals and alloys were easily oxidized.

171 Some small particles can be found within the grains in Fig. 1(b).
172 The content of each element for the particle inclusions were approxi-
173 mately 11.1 at. % in the ScYLaGdTbDyHoErLu alloy. Therefore, the
174 elemental concentration distribution within particles was analogous
175 to that of the matrix. It is worth noted that the dimension of the par-
176 ticles was beyond the resolution limit of the SEM-EDS instrument,
177 which means that the EDS spectrometer readings may contain addi-
178 tional signals from the matrix.

179 The TEM analysis was employed to further investigate the
180 composition of the particles in the ScYLaGdTbDyHoErLu alloy,
181 as displayed in Fig. 2. The morphologies of the
182 ScYLaGdTbDyHoErLu alloy were island-like in Fig. 2(a), where
183 bright precipitates were embedded in the dark matrix. The size of
184 the precipitates was approximately $1 \mu\text{m}$. The elemental composi-
185 tion of the precipitates was studied by TEM-EDS, demonstrating
186 in the upper right corner of Fig. 2(a), with a composition of
187 $\text{Sc}_{77.96}\text{Lu}_{8.4}\text{Er}_{4.76}\text{Ho}_{2.7}\text{Y}_{2.67}\text{Dy}_{1.36}\text{La}_{0.93}\text{Gd}_{0.77}\text{Tb}_{0.62}$, which mani-
188 fests that the precipitates were Sc-rich (~ 78 at. %). The TEM-EDS
189 mapping that displayed in Fig. 2(e) revealed that the precipitates
190 in the alloy mainly consisted of Sc element, which were in good
191 agreement with the results of Fig. 2(a). The SAED of the precipi-
192 tates along the $[\bar{1}12]$ zone axis was displayed in Fig. 2(c), which
193 corresponds to a BCC structure. In contrast, the XRD pattern in
194 Fig. 1(a) shows that the alloy almost has a single HCP phase, and
195 no sharp peaks corresponding to the BCC phase were captured,
196 because the small size and low volume fraction of the particles
197 were not easily detected by the XRD instrument due to the resolu-
198 tion limit.

199 Similarly, some precipitates were found in YGdTbDyHo⁴¹ and
200 YGdTbDyLu²⁰ HEAs as well. The Y-rich precipitates were mainly

located at grain boundaries in YGdTbDyHo HEAs.⁴¹ Takeuchi
et al. believed that the Ta-rich precipitates were found in the grains
of YGdTbDyLu alloys, since Ta was wrapped up by the Lu element
as a major impurity.²⁰ The different enrichment may be attributed
to many factors, such as the interaction of different constituent ele-
ments and the distinctly forming method, etc. The SAED pattern
along the $[0001]$ zone axis of the region A with an HCP structure
was shown in Fig. 2(b). The alloy was chemically homogeneous,
and there were no precipitates or secondary phases if ignoring the
presence of minor particulates inside the grains. In the as-cast
ScYLaGdTbDyHoErLu alloy, the twins were observed in Fig. 2(d).
These growth twins stemmed from nucleation along the faulted
layers during solidification.^{42–44} The width of growth twins in the
ScYLaGdTbDyHoErLu alloy mostly ranged from 100 to 300 nm.

B. Mechanical properties

The true stress–strain curve of the ScYLaGdTbDyHoErLu
alloy upon quasi-static compression is presented in Fig. 3(a).
The compressive yielding strength (σ_y^c), compressive fracture
strength (σ_f^c), and compressive plastic strain (ϵ_p^c) for the current
ScYLaGdTbDyHoErLu HEA were 251 MPa, 1197 MPa, and 20.2%,
respectively. The detailed compressive mechanical properties, the
Vickers hardness values of the ScYLaGdTbDyHoErLu HEA and its
constituent elements at room temperature are listed in Table III.

In order to explore the mechanical properties of the
ScYLaGdTbDyHoErLu HEA, the tensile tests at a strain rate of
 $5 \times 10^{-4} \text{ s}^{-1}$ at room temperature were conducted, since the tensile
strength was more sensitive to structural defects. The typical true
tensile stress–strain curves are displayed in Fig. 3(b). It can be observed
that the tensile yielding strength (σ_y^t) was 213 MPa, the tensile fracture
strength (σ_f^t) was 329 MPa, and the tensile plastic strain (ϵ_p^t) was
12.2%. It is noted that σ_f^t was much higher than σ_y^t in the current
HEA, indicating a distinguishing working-hardening capacity. The for-
mation of working hardening will be discussed in Sec. V.

For the sake of revealing deformation features of the alloy
upon quasi-static tensile deformation, TEM was employed to
observe the fracture morphology and to investigate the deformation
structure in detail. Straight line-like deformation twins (DTs) and
growth twins co-existed in the deformed alloy, as clearly observed
in Fig. 4. The inset in Fig. 4(b) was the HRTEM image of the
straight line-like DTs, and most DTs—with a twin thickness of less
than 100 nm except for the thicker growth twins were widely
found. As shown in Fig. 4(b), a large number of DTs formed along
the growth-twin walls. Meanwhile, the SAED pattern of DTs is
shown in Fig. 4(b). This result was generally consistent with previ-
ous reports that mechanical twinning was activated during continu-
ous loading in the annealed twin boundaries.⁴⁵ Under uniaxial
tensile loading, multiplication of dislocations tended to pile up at
the boundaries to form dislocation plug groups, resulting in a con-
tinuous increase in the local stress between the dislocations and
boundaries. When the local stress reached a critical value, the DTs
would be activated.

It should be noted that the growth-twin boundaries together
with grain boundaries were considered as effective barriers for dis-
locations. In addition, the dislocation interaction will lead to a
higher strain energy on the growth twins compared with the grain.

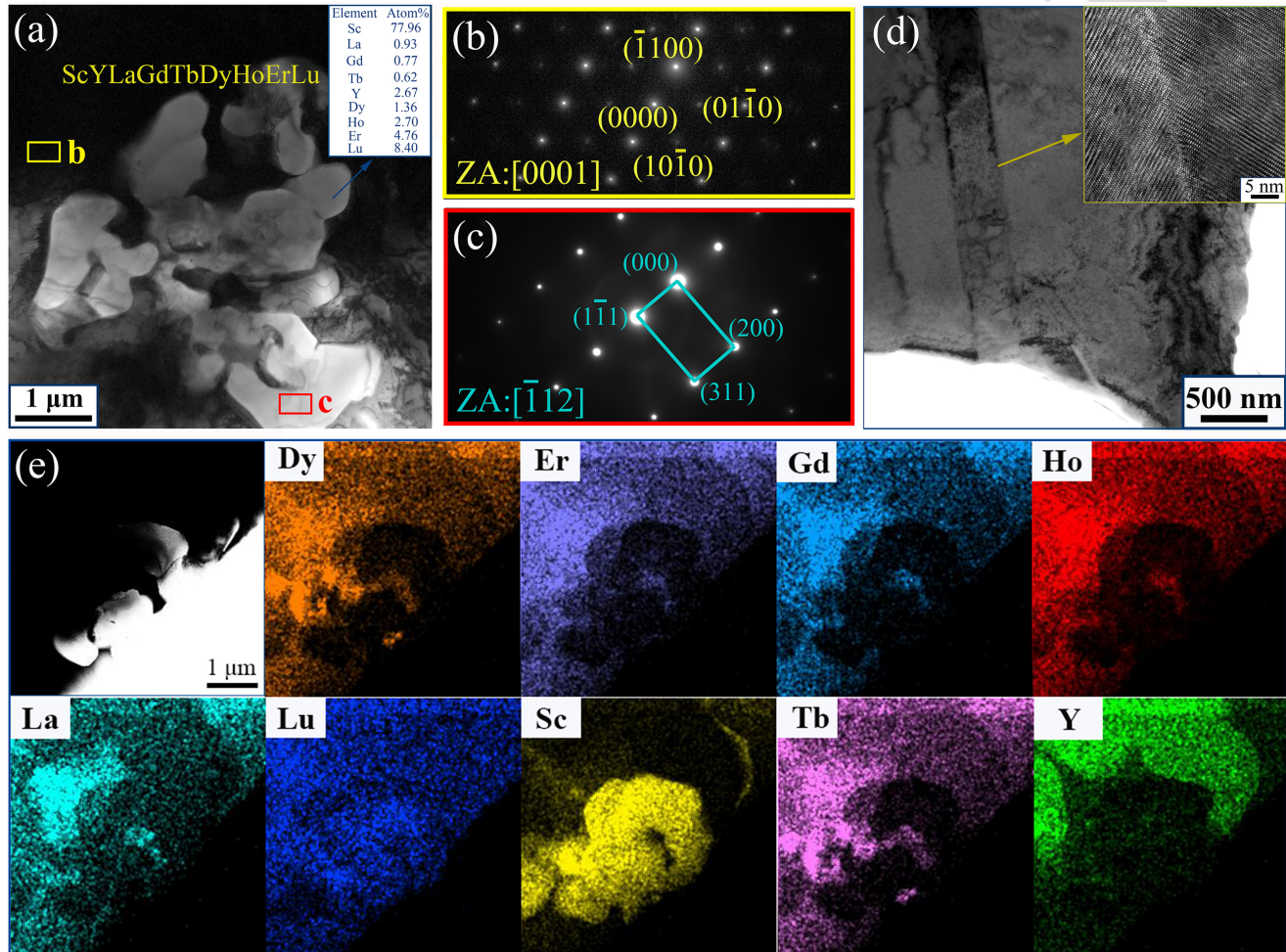


FIG. 2. (a) and (b) TEM bright-field images of the ScYLaGdTbDyHoErLu alloy for the as-cast sample in (a) and (d). (b) and (c) show SAED patterns of the precipitation and HCP matrix, respectively. TEM-EDS mappings of precipitation are shown in (e).

256 Therefore, the growth-twin boundaries acted as preferential sites by
 257 analyzing the character of DTs in the ScYLaGdTbDyHoErLu HEA.
 258 The HRTEM and inverse fast Fourier transform (IFFT) images of the
 259 bottle-shaped red wire frame that marked in Fig. 4(c) were noticeably
 260 depicted in Fig. 4(d), which reveals that there were high-density stack-
 261 ing faults (SFs) in the deformed ScYLaGdTbDyHoErLu alloy.

262 V. DISCUSSION

263 A. Rule of mixture (RoM)

264 Figure S1 shows the DSC curve of the ScYLaGdTbDyHoErLu
 265 alloy in the [supplementary material](#). A smooth curve with no endo-
 266 thermic or exothermic peaks of the HEA manifested no phase
 267 transformation appeared before it was melted. The lowest point of
 268 the curve, indicated by the arrow, is the melting point of the alloy.
 269 So it can be determined from Fig. S1 that the melting point is

1336 °C for the alloy. The ScYLaGdTbDyHoErLu alloy possesses
 high thermal stability and keeps the HCP structure all the time
 before melting. The melting points of the current HEAs and their
 constituents are listed in [Table IV](#).

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 274 Meanwhile, Poisson's ratio (ν), bulk modulus (B), Young's
 275 modulus (E), and shear modulus (G) of the alloys and the corre-
 276 sponding constituent elements are summarized in [Table IV](#).
 277 The melting point that was calculated by the rule of mixture (RoM)
 278 was 1441.6 °C, which substantially matches with the experimental
 279 values of 1336 °C. The measured elastic properties (B , E , and G)
 280 and T_m were in good agreement with the calculation by RoM. The
 281 properties (P) can be calculated by

$$P = \sum_{i=1}^n c_i P_i, \quad (6)$$

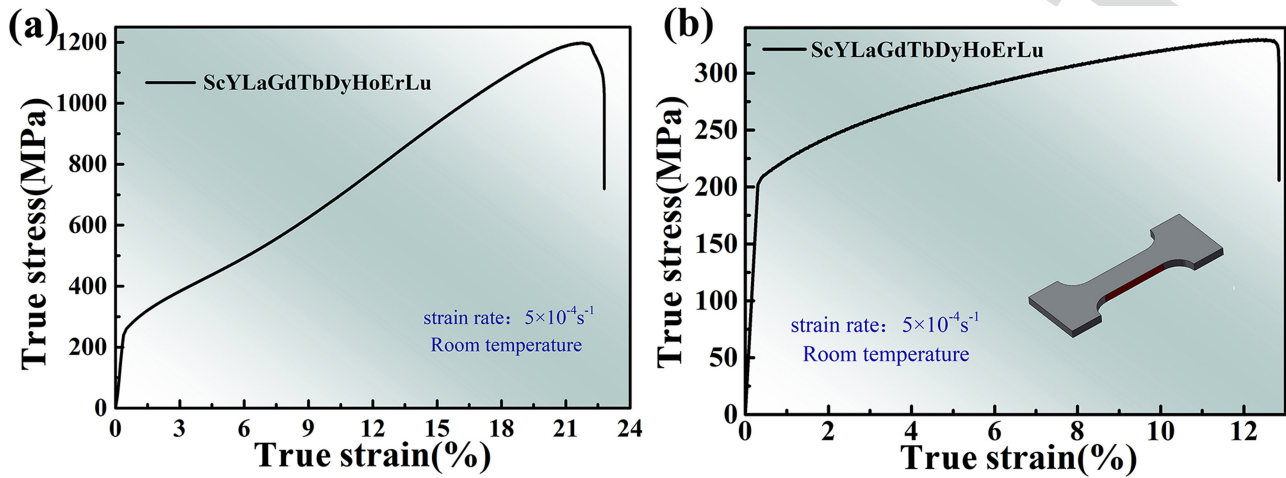


FIG. 3. (a) The compressive true stress–strain curve of the ScYLaGdTbDyHoErLu HEA at room temperature. (b) Loading the tensile true stress–strain curve of the ScYLaGdTbDyHoErLu HEA.

where P_i is the mechanical property of the constituent element. Poisson’s ratio (ν_c) of the alloys can be determined,³⁶

$$\nu_c = \frac{3B_c - 2G_c}{2(3B_c + G_c)}, \quad (7)$$

where B_c and G_c are the calculated bulk modulus and shear modulus by the RoM, respectively. ν_c of the ScYLaGdTbDyHoErLu alloy was 0.27, which is basically the same with the experimental value.

The lattice constants (a , c , and c/a ratio) of the current ScYLaGdTbDyHoErLu HEA with the constituent elements, and the calculated results by RoM, are listed in Table II. The values exhibited good agreement between the experiment and calculation. The

mechanical properties (σ_y^c and HV) of the alloy do not meet the RoM, as seen from Fig. 3(b) and Table III.

B. Solid-solution strengthening (SSS)

The Vickers hardness was linearly proportional to the compressive yielding strength, which is benefit of uncovering the strengthening mechanism based on the compressive mechanical properties. The compressive mechanical properties and hardness are summarized in Fig. 5(a). It is obvious that the experimental values have been significantly improved upon the compression yielding strength and hardness, which reveals that the present alloy has undergone vital strengthening effects. The main strengthening in most HEAs is solid-solution strengthening (SSS) since it is hard to distinguish the solute and solvent atoms. Meanwhile, the solute element content is especially high, which leads to the significant SSS results. Currently, the classical Labusch equation has been successfully modified and applied to calculate SSS in HEAs.⁴⁶ The value of SSS of the HEAs can be estimated by

$$\Delta\sigma = \left(\sum \Delta\sigma_i^{3/2} \right)^{2/3}, \quad (8)$$

where $\Delta\sigma_i$ is the SSS value of the i th component element. $\Delta\sigma_i$ can be expressed as

$$\Delta\sigma_i = ZGf_i^{4/3}c_i^{2/3}, \quad (9)$$

Here, Z is a material-dependent dimensionless constant ($Z = 0.04$),⁴⁷ G is the experimental value of the shear modulus of the HEAs, as obtained in Table IV, f_i is the mismatch parameter, as calculated in detail elsewhere,¹⁹ and c_i is the atomic fraction of the i th element.

The SSS value of the current ScYLaGdTbDyHoErLu HEA can be obtained by Eq. (11), which was 53 MPa. The SSS value was greatly enhanced with the increase in constituent elements.

TABLE III. The compression properties and hardnesses of the ScYLaGdTbDyHoErLu HEA and their constituent elements. The calculated values for HEAs are achieved by the RoM.

Alloy and elements	HV	σ_y^c (MPa)	σ_f^c (MPa)	ϵ_p^c (%)	
ScYLaGdTbDyHoErLu	Exp. cal.	164	251	1197	20.2
		98.8	169	878	25.1
Sc	...	73	55
Y	...	134	280	1065	20.6
La	...	39	90	415	34.2
Gd	...	63	83	677	25
Tb	...	71	140	921	18.6
Dy	...	110	260	823	22.3
Ho	...	127	180	976	24.2
Er	...	130	195	1233	26.9
Lu	...	142	240	915	28.9

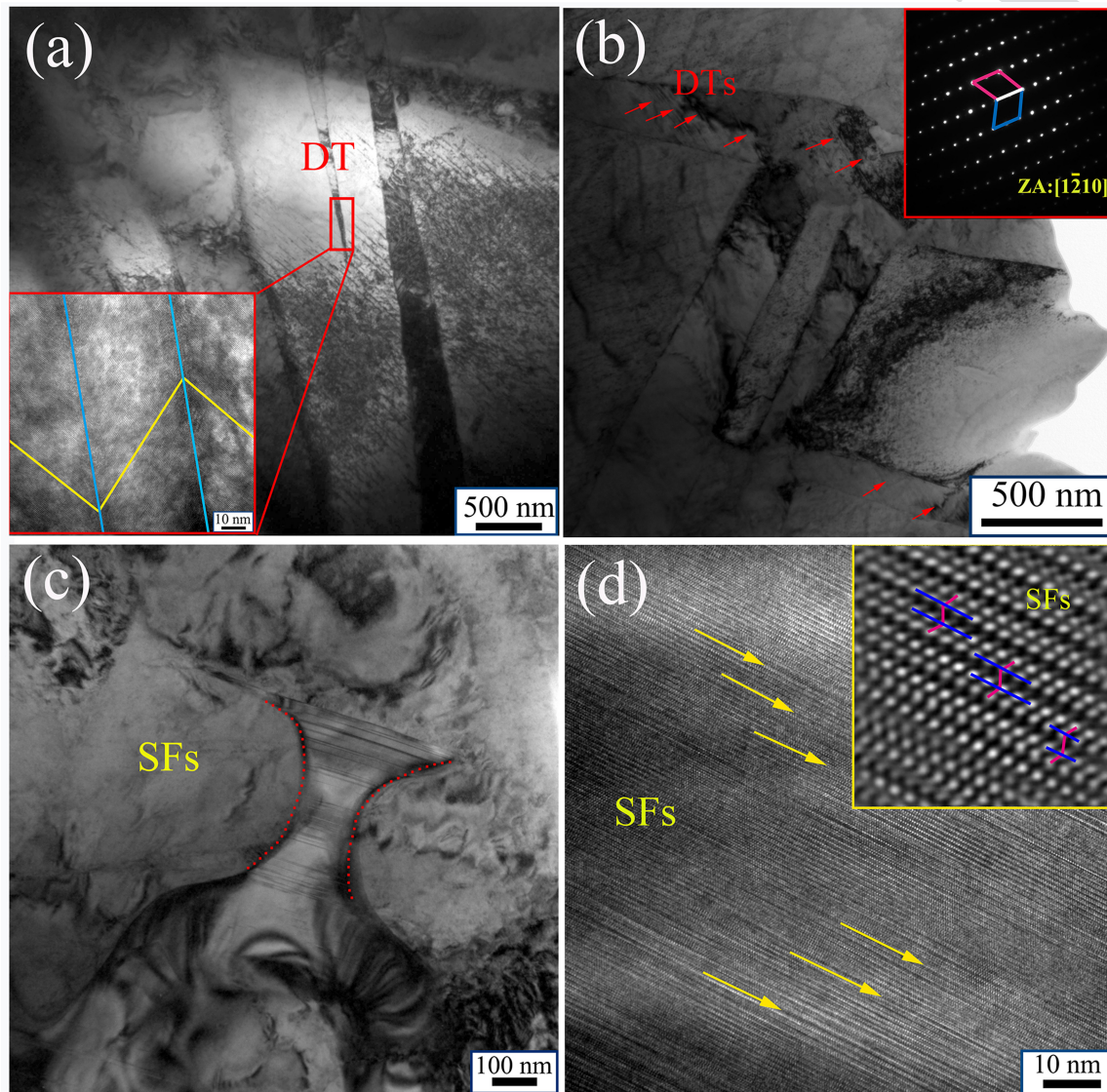


FIG. 4. (a)–(c) TEM bright-field images of the ScYLaGdTbDyHoErLu HEA after fracture. The inset in (b) is SADE patterns of TDs (the red arrow). (d) is the HRTEM of the red dashed region of (c). IFFT of the SFs is shown in the inset of (d).

317 In other words, a large lattice distortion formed a great lattice mis-
 318 match in the current rare-earth HEAs. Therefore, the larger value
 319 of δ is, the more obvious of the SSS can be obtained. More detailed
 320 values of δ and $\Delta\sigma$ in the different rare-earth HEAs are shown in
 321 Fig. 5(b). The calculated value of the compressive yielding strength
 322 (σ_y^{cal}) can be predicted by the following equation:

$$\sigma_y^{cal} = \sigma_y^{mix} + \Delta\sigma, \quad (10)$$

323 where σ_y^{mix} is the average yielding strength of the constituent ele-
 324 ments by RoM. The σ_y^{cal} value of the alloy was 222 MPa, which was

325 basically consistent with the experimental values (σ_y^e) within the
 326 allowable range of error. The calculated and experimental yielding
 327 strengths of the alloy are displayed in Fig. 5(c). Obviously, the
 328 yielding strength of the current HEA can be easily predicted by the
 329 SSS model.

C. Plastic deformation 330

331 To achieve the uniform plastic deformation and avoid crack-
 332 ing, according to the Von Mises–Taylor criterion, each grain must
 333 satisfy five independent slip systems.⁴⁸ Most of HCP alloys cannot
 334 meet the Von Mises–Taylor criterion because of lack of

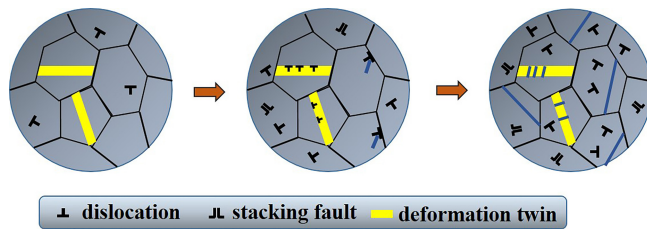


FIG. 6. The deformation processes of the ScYLaGdTbDyHoErLu HEA under quasi-static tensile.

It is obvious that the asymmetry between tensile and compressive yielding of the ScYLaGdTbDyHoErLu alloy appeared, which is related to the strength differential (SD) effect. The compressive and tensile yielding strength of the alloy were 251 and 213 MPa, respectively. The SD-parameter can be defined as^{51,52}

$$SD = 2 \frac{|CYS| - |TYS|}{|CYS| + |TYS|}, \quad (11)$$

where *CYS* and *TYS* represent the compressive yielding stress and tensile yielding stress, respectively. *CYS* was slightly higher than the *TYS* in the ScYLaGdTbDyHoErLu alloy, and the *SD* value was 0.1638. In other words, the tension-compression yielding asymmetry of the alloy existed under the uniaxial stress state at room temperature.

Generally, the tension-compression yielding asymmetry phenomenon has been widely reported in many traditional alloys, such as magnesium alloys^{53,54} and aluminum alloys.⁵⁵ The pronounced negative *SD* effect takes place in most conventional alloys in which the *CYS* is significantly lower than the *TYS*.^{51,56} This rare-earth based HEA has nonequivalent families of slip systems, since the HCP structure is geometrically anisotropic and the critical resolved shear stress on the slip system changes considerably. Compared with FCC or BCC alloys, the current HCP HEA deformed by slip and twinning during the plastic deformation. Different from non-directional slips, twinning is more sensitive to the shear direction, which means the twinning can be active in one direction but not activated in the opposite direction. According to the TEM results, a large number of DTs can be observed after fracture. The DTs will be activated during the plastic deformation due to the high level of local stress. In the current HCP HEA, the basal slip and twinning played a more significant role in the compression tests. However, the basal slip and non-basal slip were regarded as the main deformation mechanism in tension.⁵⁷ The higher *CYS* was obtained because of the difference of critical activation stress of non-basal slips and twinning, which results in the asymmetry in tension and compression tests.

VI. CONCLUSIONS

In summary, a novel ScYLaGdTbDyHoErLu alloy with a single HCP structure was designed, as predicted by the proposed parameters, including ΔH_{mix} , ΔS_{mix} , δ , VEC, and φ -parameter. The

microstructures and mechanical properties were investigated in detail, from which the main conclusions were obtained as follows:

- (1) The thermodynamic parameters were used to preliminarily predict the single HCP phase of the ScYLaGdTbDyHoErLu rare-earth based HEA, which was verified by SEM and TEM characterization.
- (2) The lattice constants, melting point, and elastic properties (bulk modulus, Young's modulus, and shear modulus) of the ScYLaGdTbDyHoErLu alloy that were obtained were in accordance with the RoM. The hardness and compressive yielding strength that calculated by RoM were higher than the experimental values, which reveals the obvious strengthening effect.
- (3) The compressive yielding strength of the HEA can be well predicted by the SSS model. The value of $\Delta\sigma$ of the ScYLaGdTbDyHoErLu alloy was 53.29 MPa. The solid-solution strengthening effect will be stronger due to the increase in compositional element or difference in atomic radii.
- (4) A large number of SFs and DTs nucleated from the growth-twin boundaries by observing the morphologies of tensile specimens. The asymmetry phenomenon was characterized by the positive *SD* parameter, since the compressive yielding strength was higher than the tensile yielding strength in the current HEA.

SUPPLEMENTARY MATERIAL

See the [supplementary material](#) for the DSC curve of the ScYLaGdTbDyHoErLu HEA. The melting point of the current alloy was marked by the red arrow in Fig. S1.

AUTHORS' CONTRIBUTIONS

Z.W. and M.L.B. contributed equally to this work.

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DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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