High-throughput search for RE (La, Ce and Y) contained stoichiometric compound in steels

Cainv Ma1, Meng Lv1, Xueyun Gao1, Haiyan Wang1,∗, Huihui Wei1,3,4 and Shiyi Gao1,∗

1 School of Materials and Metallurgy, Inner Mongolia University of Science and Technology, Baotou 014010, People’s Republic of China
2 Key Laboratory of Integrated Exploitation of Bayan Obo Multi-Metal Resource , Inner Mongolia University of Science and Technology, Baotou 014010, People’s Republic of China
3 Inner Mongolia Baotou Steel Union Co., Ltd., Baotou 014010, People’s Republic of China
4 Inner Mongolia Enterprise Key Laboratory of Rare Earth Steel Products Research and Development, Baotou 014010, People’s Republic of China
5 Key Laboratory of Modern Welding Technology of Guangdong Province, China-Ukraine Institute of Welding, Guangdong Academy of Sciences, Guangzhou 510650, People’s Republic of China

∗ Authors to whom any correspondence should be addressed.

E-mail: windflower126@163.com and meshiyigao@163.com

Keywords: high-throughput search, rare earth, compounds, steels

Abstract

The design of rare earth (RE) bearing steels requires a thorough understanding of the formation tendency of RE involved phases in steels, while searching for binary and ternary compounds with a wide variety of composition and permutation need a remarkable amount of experimentation which is nearly infeasible. In the present work, we perform a thorough search for the RE-contained compounds in steels by a data-driven high-throughput computational approach. The search results indicate that RE may react with O and N to form a large amounts of oxide and nitride inclusions, while only Y can participate in the formation of sulfi de inclusion Y2MnS4 and Y2CaS4. For the case of ternary compounds in Fe-based solid solution, it is found that RE prefers to form ternary phases with the non-metallic elements, i.e., B, C, O, P and Si, and only Y is found to combine with metal Cr to form YCr4Fe8. Finally, our screen suggests that RE can participate in the formation of the nano-scale precipitates of κ-carbides, L12 precipitates and B2 precipitates, but MC and M2C carbides.

1. Introduction

In recent years, rare earth (RE) elements addition has received increasing interest in steel metallurgy. A series of benefi cial research for the development of RE-bearing steels have been focused on the purifi cation and modifi cation of inclusions since RE elements are characterized by signifi cant negative free energy changes for compound formations [1, 2]. It has been reported that RE elements exhibit a remarkable ability to reduce oxygen and sulfur content to a magnitude of 10−6, and the addition of RE elements results in a considerable change in inclusion composition and the formation of RE-contained oxides and sulfi des [3, 4]. RE elements can also dissolve in Fe matrix to form a solid solution, and thus affect the formation kinetics of precipitates and the phase transition due to their interactions with the defects, i.e. vacancy, dislocation and grain boundary, and other alloy elements [5, 6]. Moreover, studies have shown that RE addition also improves the high-temperature oxidation resistance and corrosion resistance due to the reactive-element eff ect [7, 8].

Although the effects of RE on the microstructure and properties have been investigated widely, the reported results of RE-involved compounds are so far focused in the inclusion formation during the steel-making process [9, 10]. Further applications of RE elements in steels will require more acknowledgments of the existing state of RE elements and the discovery of RE-contained compounds in the steel system. However, a systematic search for the RE-contained compounds for a wide variety of solutes using brute force experimentation is infeasible.

The first-principles calculations have been employed in materials science for years, and have already exhibited the potential to greatly accelerate the design and prediction of new materials without having to
synthesize them in advance. The past years have seen the emergence of many databases for materials properties from the first-principles calculations [11–16]. With advances in computational resource, the high-throughput computational method has been developed to increase computational efficiencies. So far, there are several remarkable efforts that use high-throughput first-principles calculations of compounds from large crystal structure databases for materials prediction and design, i.e. the Python Materials Genomics (Pymatgen) [17], Open Quantum Materials Database (OQMD) [18] and Automatic Flow (AFLOW) [19] software frameworks. Indeed, these frameworks have been successfully applied in the search for materials such as Li-ion batteries, alloys, intermetallics and inorganic compounds [20–22].

In the present work, to identify the formation preferences of the commonly used RE (La, Ce and Y) elements in steels, we perform a high-throughput search for the RE-contained compounds in steels refers to the inclusions, Fe-based solid solution and nano-sized precipitates.

2. Methodology

The objective of the present work is to identify compounds of being composed of RE (La, Ce and Y) elements that are likely to form in steels. We utilize the OQMD to search the corresponding compounds. The OQMD is a high-throughput DFT (Density functional theory) database which contains approximately 300,000 DFT total energy calculations of compounds from the Inorganic Crystal Structure Database (ICSD) and decorations of common crystal structures [18]. All the calculations were performed using the projector-augmented wave (PAW) method as implemented in the Vienna Ab initio Simulation Package (VASP) [23, 24] with the Perdew–Burke–Ernzerhof (PBE) exchange-correlation function of the generalized gradient approximation (GGA) [25]. Spin-polarized calculations were included for all calculations and the cutoff energy for plan-wave was 520 eV. The Brillouin zone integrations were performed using a Gamma scheme with at least 8,000 k-points per unit cell. Electronic minimization was done with Gaussian smearing of width 0.2 eV by setting the convergence criterion to $10^{-5}$ eV atom$^{-1}$, whereas, ionic relaxation was performed using conjugate-gradient algorithm with a force criterion of 0.02 eV/Å.

To search the reasonable candidate compounds, these compounds must be stable or nearly stable. By calculating the formation energies of all the competing phases of a concerned chemical system, one can build a formation energy-composition phase diagram, in which a so-called convex hull is constructed by creating a calculating the formation energies of all the competing phases of a concerned chemical system, one can build a convex hull is constructed by creating a

$$
\Delta H_f = E(A_{m}B_{n}C_{l}) - [x_{A}E(A) + x_{B}E(B) + x_{C}E(C)]
$$

where the formation energy is given by the energy of $A_{m}B_{n}C_{l}$ relative to the composition-weighted $(x_{A}, x_{B}$ and $x_{C}$) average of the energies of the pure constituents each in their equilibrium crystal structures. $E(A_{m}B_{n}C_{l})$, $E(A)$, $E(B)$ and $E(C)$ are the energies (per atom ) of the compound $A_{m}B_{n}C_{l}$ and constituents A, B and C, respectively. In the present paper, we consider the phases with formation energies on the convex hull ($\Delta H_{f, stab} = 0$) and those within 25 meV atom$^{-1}$ above the convex hull (nearly stable, $\Delta H_{f, stab} \leq 25$ meV atom$^{-1}$) are more likely to form in our system. In the present work, we concentrate on the search for RE-containing stoichiometric compounds, and the non-stoichiometric compounds which involve RE atoms that randomly distribute on the host lattice to form random substitutional phases are not explored.

3. Results and analysis

3.1. RE contained inclusions

3.1.1. Oxide inclusions

For RE participating in the formation of oxide inclusions, we performed the search for that involved with the common oxide inclusions in steel-making process, i.e., aluminum oxide, silicon oxide, manganese oxide, chromium oxide, titanium oxide and iron oxide. Figure 1(a) presents the ternary phase diagram of Al-O-La, in which the red dots represent the stable compounds, and green dots represent the nearly stable compounds. As shown in figure 1(a), La may form La2O3 and LaAlO3 with oxygen, and these two oxides (or one of them) react with Al2O3 (or LaAlO3) to form LaAlO3. The space group of LaAlO3 is R3c and the corresponding crystal structure is illustrated in figure 1(b), and its calculated formation energy is 3.561 eV atom$^{-1}$ as listed in the first line of table 1. Table 1 presents the predicted RE-contained oxide inclusions along with the corresponding space groups, formation energies, distances from the convex hull and formation reactions. It can be seen that La, Ce and Y can all form oxide inclusions with Al, Si, Mn, Cr, Ti and Fe, respectively, and the number of oxides that can be formed is 34, in which YAlO3, LaMn7O12, LaTiO3 and Y3Fe5O12 are nearly stable. Among these oxide
Figure 1. Calculated phase diagram for La-Al-O ternary system (a) and the illustration of conventional crystal structure of LaAlO$_3$ (b). In the phase diagram, the stable and nearly stable compounds are denoted as red and green dots, respectively, and the stable phases are connected by black tie-lines to form the convex hull.

Table 1. Oxide inclusions containing RE (La, Ce or Y) elements, in which $\Delta H_f$ denotes the formation energy and $\Delta H_{stab}$ represents the distance between the formation energy and the ground state convex hull.

| Compound        | Space group | $\Delta H_f$ (eV atom$^{-1}$) | $\Delta H_{stab}$ (eV atom$^{-1}$) | Reaction                                           |
|-----------------|-------------|--------------------------------|------------------------------------|---------------------------------------------------|
| AlO-contained   |             |                                |                                    |                                                   |
| LaAlO$_3$       | R3c         | $-3.561$                       | 0                                  | La$_2$O$_3$(or La$_3$O$_4$)+Al$_2$O$_3$(or LaAl)$_3$+O |
| CeAlO$_3$       | R3c         | $-3.479$                       | 0                                  | Ce$_2$O$_3$(or Ce$_3$O$_4$)+Al$_2$O$_3$(or CeAl)$_3$+O |
| YAlO$_3$        | Pnma        | $-3.560$                       | 0.017                              | Y$_2$O$_3$+ Al$_2$O$_3$                           |
| Y$_2$Al$_2$O$_7$| Ia3d        | $-3.519$                       | 0                                  | YO$_2$(or Y$_2$O$_3$)+Al$_2$O$_3$(or YAl)$_3$+O    |
| SiO-contained   |             |                                |                                    |                                                   |
| La$_2$SiO$_3$   | P21/c       | $-3.606$                       | 0                                  | La$_2$O$_3$(or La$_3$O$_4$)+Si$_2$O$_3$(or LaSi)$_2$+O + Si |
| La$_2$Si$_2$O$_7$| P1          | $-3.479$                       | 0                                  | La$_2$O$_3$+ Si$_2$O$_3$ + O + Si                 |
| Ce$_2$Si$_2$O$_7$| P21/c       | $-3.492$                       | 0                                  | Ce$_2$O$_3$(or Ce$_3$O$_4$)+Si$_2$O$_3$(or CeSi)$_2$+O + Si |
| Ce$_2$Si$_3$O$_7$| P41         | $-3.411$                       | 0                                  | Ce$_2$O$_3$+ Si$_2$O$_3$ + O + Si                 |
| Y$_2$Si$_2$O$_7$| C2/c        | $-3.600$                       | 0                                  | YO$_2$(or Y$_2$O$_3$)+Si$_2$O$_3$ + O + Si       |
| Y$_2$Si$_3$O$_7$| C2/m        | $-3.492$                       | 0                                  | YO$_2$(or Y$_2$O$_3$)+Si$_2$O$_3$ + O + Si       |
| MnO-contained   |             |                                |                                    |                                                   |
| LaMnO$_3$       | Pnma        | $-2.932$                       | 0                                  | La$_2$O$_3$+ Mn$_2$O$_3$(or Mn$_3$O$_4$, Mn$_2$O$_6$, MnO) |
| LaMn$_2$O$_5$   | Pnma        | $-2.562$                       | 0                                  | La$_2$O$_3$(or La$_3$O$_4$)+Mn$_2$O$_3$(or Mn$_2$O$_6$, Mn$_3$O$_4$)+O |
| LaMn$_3$O$_7$   | C2/m        | $-2.244$                       | 0.011                              | La$_2$O$_3$(or La$_3$O$_4$)+Mn$_2$O$_3$(or Mn$_3$O$_4$) |
| CeMnO$_3$       | Pnma        | $-2.848$                       | 0                                  | Ce$_2$O$_3$(or Ce$_3$O$_4$)+Mn$_2$O$_3$(or Mn$_2$O$_6$, Mn$_3$O$_4$)+O |
| CrO-contained   |             |                                |                                    |                                                   |
| LaCrO$_3$       | Pnma        | $-3.168$                       | 0                                  | La$_2$O$_3$(or La$_3$O$_4$)+Cr$_2$O$_3$(or Cr$_3$O$_4$)+O + Cr |
| LaCr$_2$O$_4$   | Fddd        | $-2.737$                       | 0                                  | La$_2$O$_3$(or La$_3$O$_4$)+Cr$_2$O$_3$(or Cr$_3$O$_4$)+O + Cr |
| La$_2$CrO$_6$   | C2/c        | $-2.930$                       | 0                                  | La$_2$O$_3$(or La$_3$O$_4$)+Cr$_2$O$_3$(or Cr$_3$O$_4$)+O + Cr |
| CeCrO$_3$       | Pnma        | $-3.082$                       | 0                                  | Ce$_2$O$_3$(or Ce$_3$O$_4$)+Cr$_2$O$_3$(or Cr$_3$O$_4$)+O + Cr |
| CeCr$_2$O$_4$   | I41/        | $-2.651$                       | 0                                  | Ce$_2$O$_3$(or Ce$_3$O$_4$)+Cr$_2$O$_3$(or Cr$_3$O$_4$)+O + Cr |
|                 | amd         |                                |                                    |                                                   |
| YCrO$_3$        | Pnma        | $-2.114$                       | 0                                  | YO$_2$(or Y$_2$O$_3$)+Cr$_2$O$_3$(or Cr$_3$O$_4$)+O + Cr |
| YCr$_2$O$_4$    | I41/        | $-3.178$                       | 0                                  | YO$_2$(or Y$_2$O$_3$)+Cr$_2$O$_3$(or Cr$_3$O$_4$)+O + Cr |
| TiO-contained   |             |                                |                                    |                                                   |
| La$_2$TiO$_3$   | Pnma        | $-3.465$                       | 0.010                              | La$_2$O$_3$(or La$_3$O$_4$)+Ti$_2$O$_3$            |
| La$_2$Ti$_2$O$_5$| P21         | $-3.573$                       | 0                                  | La$_2$O$_3$(or La$_3$O$_4$)+Ti$_2$O$_3$(or Ti$_2$O$_3$, Ti$_3$O$_4$)+O |
| CeTiO$_3$       | Pnma        | $-3.363$                       | 0                                  | Ce$_2$O$_3$+ Ti$_2$O$_3$(or Ti$_3$O$_4$, Ti$_2$O$_3$, Ti$_3$O$_4$) |
| Y$_2$TiO$_3$    | Pnma        | $-3.663$                       | 0                                  | YO$_2$(or Y$_2$O$_3$)+Ti$_2$O$_3$(or Ti$_2$O$_3$, Ti$_3$O$_4$, TiO)$_3$+O |
| FeO-contained   |             |                                |                                    |                                                   |
| LaFeO$_3$       | Pnma        | $-2.755$                       | 0                                  | La$_2$O$_3$(or La$_3$O$_4$)+Fe$_2$O$_3$(or Fe$_2$O$_3$, FeO)$_3$+O + Fe |
| La$_2$Fe$_2$O$_5$| Cmc21       | $-3.234$                       | 0                                  | La$_2$O$_3$(or La$_3$O$_4$)+Fe$_2$O$_3$(or Fe$_2$O$_3$, FeO)$_3$+O + Fe |
| CeFeO$_3$       | Pnma        | $-2.669$                       | 0                                  | Ce$_2$O$_3$(or Ce$_3$O$_4$)+Fe$_2$O$_3$(or Fe$_2$O$_3$, FeO)$_3$+O + Fe |
| YFeO$_3$        | Pnma        | $-1.543$                       | 0                                  | YO$_2$(or Y$_2$O$_3$)+Fe$_2$O$_3$(or FeO)$_3$+O + Fe |
| Y$_2$Fe$_2$O$_7$| Ia3d        | $-2.458$                       | $-0.023$                           | YO$_2$(or Y$_2$O$_3$)+Fe$_2$O$_3$+O + Fe |

The calculated properties are based on the electronic structure calculations performed using the density functional theory (DFT) method within the generalized gradient approximation (GGA) framework. The structures were optimized using the Perdew-Burke-Ernzerhof (PBE) exchange-correlation functional.
inclusions, LaAlO3 and CeAlO3 inclusions have been confirmed in steel-making process by Wang and Yu et al [27, 28]. Additionally, the R3c space group only observed in AlO-contained system, and Pnma space group is the most common structure for the RE-contained oxide inclusions.

### 3.1.2. Sulphide inclusions

For RE participating in the formation of sulphide inclusions, we performed the search for the compounds involved with manganese sulphide, iron sulphide and calcium sulphide. As shown in table 2, the results indicate that none of the three RE elements (La, Ce and Y) exhibits a preference for forming stable (or nearly stable) compounds with FeS. For MnS and CaS, only Y element is found to react with them and the products are Y2MnS4 and Y2CaS4, respectively, in which Y2CaS4 is nearly stable. Although it has been reported that La2Fe2S5 with a space group of Cmc21 can be prepared from the reaction of La2S3 and FeS at 1223 K [29], the calculations reveal that its formation energy is 0.131 eV atom$^{-1}$ above the convex hull. Therefore, compared with Y2MnS4 and Y2CaS4, it is considered that La2Fe2S5 is difficult to be formed at 0 K. The phase diagrams of Y-Mn-S and Y-Ca-S, and the conventional crystal structures of the two phases Y2MnS4 (c) and Y2CaS4 (d), respectively.

![Figure 2. Calculated phase diagrams for Y-Mn-S (a) and Y-Ca-S (b) ternary systems, and the illustrations of conventional crystal structures of Y2MnS4 (c) and Y2CaS4 (d), respectively.](image)

| Compound          | Space group | $\Delta H_f$ (eV atom$^{-1}$) | $\Delta H_{stab}$ (eV atom$^{-1}$) | Reaction              |
|-------------------|-------------|-------------------------------|-----------------------------------|-----------------------|
| MnS-contained     | Y2MnS4      | 1.806                         | 0                                 | Y2S3 + MnS + Mn       |
| FeS-contained     | —           | —                             | —                                 | —                     |
| CaS-contained     | Y2CaS4      | 2.273                         | 0.006                             | Y2S3 + CaS            |

### 3.1.3. Nitride inclusions

For RE participating in the formation of nitride inclusions, we performed the search for the compounds involved with titanium nitride, niobium nitride, vanadium nitride, and aluminum nitride. As shown in table 3, TiN can only react with La to form La3Ti2N6 with I4/mmm space group, and NbN can react with La and Ce to
form La₃Nb₂N₆ and Ce₃Nb₂N₆ with also I₄/mmm space group. Both VN and AlN can react with the three RE elements, and the compounds formed by the former and REs are all I₄/mmm structure while the compounds formed by the latter and REs are all Pm₃m structure.

### 3.2. Ternary compounds in Fe-based solid solution

For the formation of ternary phases in Fe matrix, these phases need to be in equilibrium with the host lattice [22]. In other words, if a phase is not in equilibrium with the host phase, it will be excluded from consideration even if it is stable. The equilibrium state between a ternary compound and host phase (in this case, it refers to Fe) is determined by calculating the convex hull around the compound and the host phase, and examining if there is a tie-line between these two phases. This approach is illustrated in figure 3. Figure 3(a) shows that CeFe₄B₄ is a stable phase but not in equilibrium with Fe matrix because there is not a tie-line between CeFe₄B₄ and Fe, the blue dashed line refers to a non-existent tie-line. On the other hand, figure 3(b) indicates that CeFeC₂ is connected with Fe by a tie-line which suggests that the addition of small amounts of C and Ce to Fe should give rise to the formation of a two-phase equilibrium between CeFeC₂ and Fe matrix.

Table 4 lists the ternary precipitation compounds (RE-Fe-X) associated with the common non-metallic elements (X) in steels which are predicted to be formed in Fe-based alloy system. It can be seen that N has no tendency to form stable second phases with RE and Fe. Among the rest of the concerned non-metallic elements, i.e., B, C, O, P and Si, B can react with La and Y to form La₂Fe₁₄B and Y₂Fe₁₄B with P42/nmm crystal structure which are the common phase in rare earth permanent magnet materials [30], and C, P and Si exhibit a tendency to form precipitates with all the three RE elements. For Ce-Fe-Si ternary system, the stable phases CeFeSi and CeFe₅Si₂ have also been confirmed by Berthebaud et al [31] in their phase diagram experiments. Additionally, in the search for the common metallic elements involved ternary precipitations, our results reveal that only Cr can combine with Y to produce YCr₄Fe₆ with I₄/mmm crystal structure.

**Table 3.** Nitride inclusions containing RE (La, Ce or Y) elements, in which ΔHₚ denotes the formation energy and ΔHstab represents the distance between the formation energy and the ground state convex hull.

| Compound          | Space group | ΔHₚ(eV atom⁻¹) | ΔHstab(eV atom⁻¹) | Reaction                                                                 |
|-------------------|-------------|----------------|-------------------|--------------------------------------------------------------------------|
| TiN-contained     | I₄/mmm      | −1.505         | 0                 | LaN₂(or LaN)+TiN                                                        |
| NbN-contained     | I₄/mmm      | −1.414         | 0                 | LaN₂(or LaN)+Nb₅N₆(or NbN, Nb₂N)                                         |
| VN-contained      | I₄/mmm      | −1.417         | 0                 | LaN₂(or LaN)+VN(or V₂N)                                                 |
| AlN-contained     | Pm₃m        | −0.806         | 0                 | LaN + LaAl(or LaAl₂)+La                                                 |
| Ce₃AlN            | Pm₃m        | −0.713         | 0                 | CeN + CeAl(or CeAl₂)+Ce                                                 |
| Y₃AlN             | Pm₃m        | −0.975         | 0                 | YN + Y₂Al(or Y₂Al₂)+Y                                                   |

![Figure 3. Illustration of two-phase equilibrium criterion based on the tie-line connection, (a) Fe-B-Ce and (b) Fe-C-Ce ternary systems. The blue dashed line denotes a non-existent tie-line.](image-url)
3.3. Nano-Scale Precipitates

Precipitation hardening is one of the effective techniques to design advanced steels with superior strength characteristics. In recent years, nano-sized precipitation strengthened steels have received increasing interest because of their remarkable mechanical behaviors, such as excellent creep resistance, high specific strength to weight ratio, outstanding combination of strength and ductility. In this section, we explore the possibility of RE (La, Ce and Y) participating in the formation of nano-scale intermetallic precipitates in steels.

As presented in the first column of table 5, the recently investigated intermetallic precipitates in steels that exhibit fascinating strengthening and toughening effects at the nanometer scale are κ-carbides, MC carbides, M2C carbides, L12 precipitates, B2 precipitates, and L21 precipitates. So, To identify RE-compounds that can strengthen steel effectively by precipitation strengthening effect, we searched based on the above precipitation prototypes. In the case of solid phase transitions in metal, it is often found that a metastable phase is formed and maintained for a relatively long period, such as γ precipitation phase (space group P3m1) in Mg-Y-Zn system which is 168 meV atom$^{-1}$ above the convex hull. Therefore, we raise the stability threshold from 25 meV atom$^{-1}$ to 300 meV atom$^{-1}$ in this section.

As shown in table 5, the search results indicate that these three RE elements don’t prefer to form MC and M2C type carbides. Y can combine with Al and C to form a κ-carbides precipitate Y3AlC ($\Delta H_{stab} = 0$ eV atom$^{-1}$), and with Ni to form L12 type precipitate Ni3Ti ($\Delta H_{stab} = 0.183$ eV atom$^{-1}$). On the other hand, La, Ce and Y all show the tendency to participate in the formation of B2 and L21 precipitates with the corresponding stoichiometric ratio. Based on the reported experimental investigations in metals, we may conclude that RE elements are more
inclined to form the predicted precipitates with a site occupancy, e.g., partially disordered B2 La$_{1-x}$Ni$_x$Al$_x$ instead of ordered B2 LaAl or LaNi, while this site preference of RE in the precipitates need more detailed investigations in future.

4. Conclusions

In the present work, we present a comprehensive search for compounds involved with RE (La, Ce and Y) elements in steels through a high-throughput computational approach. The candidate compounds were determined based on their stability which is associated with the corresponding distance of formation energy from the ground state convex hull, and the predicted results provide the compounds in stable equilibrium, or in nearby stable state which are likely to form as metastable phases. The results indicate that RE may react with O and N to form a large amounts of oxide and nitride inclusions, while for sulfide inclusions only Y participate in the formation of Y$_2$MnS$_4$ and Y$_2$CaS$_4$. For the search for ternary compounds in Fe-based solid solution, we take into account the two-phase equilibrium between the considered compounds and Fe matrix, and the results reveal that RE prefers to form ternary phases with the non-metallic elements, i.e., B, C, O, P and Si, while only Y is found to combine with metal Cr to form YCr$_4$Fe$_8$. Finally, our screen suggests that RE can participate in the formation of the nano-scale precipitates of r-carbides, L1$_2$ precipitates and B2 precipitates, but MC and M$_2$C carbides.

Acknowledgments

The authors are grateful for the financial support of the National Natural Science Foundation of China (No. 519610130), National Science Foundation of Inner Mongolia (No. 2019MS05013), Inner Mongolia Major Basic Research Open Project (No. 0460691701), Youth innovation Talent Project of Baotou, and the Central government guides local science and technology development fund projects of China.

Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

ORCID iDs

Haiyan Wang https://orcid.org/0000-0003-3565-0196

References

[1] Torkamani H, Raygan S, Garcia-Mateo C, Rassizadehghani I, Palizdar Y and San-Martín D 2018 Metall. Mater. Trans. A 49 4495–8
[2] Torkamani H, Raygan S, Mateo C, Rassizadehghani I, Vivas I, Palizdar Y and San-Martín D 2017 Metals 7 377
[3] Pan F, Zhang J, Chen H L, Su Y H, Kuo C L, Su Y H, Chen S H, Lin K J, Hsieh P H and Hwang W S 2016 Materials 9 417
[4] Deng X, Jiang M and Wang X 2012 Acta Metall. Sin. 25 241–8
[5] Gao X, Ren H, Wang H and Chen S 2017 Mater. Sci. Eng. A 683 116–22
[6] Chen L, Ma X, Jin M, Wang J, Long H and Mao T 2015 Metall. Mater. Trans. A 47 33–8
[7] Thanneeru R, Patil S, Deshpande S and Seal S 2017 Acta Mater 55 3457–66
[8] Liu C, Revilla R I, Liu Z, Zhang D, Li X and Terryn H 2017 Corros. Sci. 129 82–90
[9] Wei W, Wu K, Zhang X, Liu J, Qiu P and Cheng L 2020 J. Mater. Res. Technol. 9 1412–24
[10] Yang C, Luan Y, Li J and Li Y 2019 J. Mater. Sci. Technol. 35 1298–308
[11] Hill J, Mulholland G, Persson K, Seshadri R, Wolverton C and Meredith B 2016 MRS Bull. 41 399–409
[12] Setyawan W and Curtarolo S 2010 Comput. Mater. Sci. 49 299–312
[13] Setyawan W, Gaume R M, Lam S, Feigelson R S and Curtarolo S 2011 ACS Comb. Sci. 13 382–90
[14] Landis D D, Hummelshøj J S, Nesterov S, Greeley J, Dullak M, Bilgaard T, Norrak J K and Jacobsen K W 2012 Comput. Sci. Eng. 14 51–7
[15] Jain A et al 2013 APL Mater. 1 011102
[16] Saal J E, Kirklin S, Aykol M, Meredith B and Wolverton C 2013 JOM 65 1501–9
[17] Ong S P, Richards W D, Jain A, Hautier G, Kocher M, Cholia S, Gunter D, Chevrier V L, Persson K A and Ceder G 2013 Comput. Mater. Sci. 68 314–9
[18] Kirklin S, Saal J E, Meredith B, Thompson A, Doak J W, Aykol M, Rühl S and Wolverton C 2015 npj Comput. Mater. 1 15010
[19] Curtarolo S et al 2012 Comput. Mater. Sci. 58 218–26
[20] Mueller T, Hautier G, Jain A and Ceder G 2011 Chem. Mater. 3 3854–62
[21] Ozolins V, Majzoub E H and Wolverton C 2009 J. Am. Chem. Soc. 131 230–7
[22] Kirklin S, Saal J E, Hegde V I and Wolverton C 2016 Acta Mater 102 125–35
[23] Kresse G and Joubert D 1999 Phys. Rev. B 59 1758
[24] Blöchl P E 1994 Phys. Rev. B 50 17953
[25] Wang Y and Perdew JP 1991 Phys. Rev. B 44 13298
[26] Kim K, Zhou B C and Wolverton C 2018 Acta Mater. 145 337–46
[27] Wang H, Yu P, Jiang S, Bai B, Sun L and Wang Y 2020 Metals 10 275
[28] Yu Z and Liu C 2019 Metals 9 804
[29] Mitchell K and Ibers JA 2002 Chem. Rev. 102 1929
[30] Yao Q, Shen Y, Yang P, Zhou H, Rao G, Deng J, Wang Z and Zhong Y 2016 J. Rare Earths 34 1121–5
[31] Berthebaud D, Touguiat O, Potel M and Noel H 2007 J. Alloys Compd. 442 104–7
[32] Sun L et al 2018 Acta Mater 149 285–301
[33] Song G et al 2015 Sci. Rep. 5 16327
[34] Song G, Sun Z, Clausen B and Liaw P K 2017 J. Alloys Compd. 693 921–8
[35] Yao M J, Dey P, Seol J B, Choi P, Herbig M, Marceau R K W, Hickel T, Neugebauer J and Raabe D 2016 Acta Mater. 106 229–38
[36] Kamikawa N, Hirohashi M, Sato Y, Chandiran E, Miyamoto G and Furuhara T 2015 ISIJ Int. 55 1781–90
[37] Liu H, Zhu J, Lai Z, Zhao R and He D 2009 Scripta Mater 60 949–52
[38] Zhang B B, Yan F K, Zhao M J, Tao N R and Lu K 2018 Acta Mater 151 310–20
[39] Teng Z K, Miller M K, Ghosh G, Liu C T, Huang S, Russell K F, Fine M E and Liaw P K 2010 Scripta Mater 63 61–4
[40] Song G, Hong S J, Lee J K, Song S H, Hong S H, Kim K B and Liaw P K 2019 Scripta Mater 161 18–22
[41] Wang D, Amstler M, Hepple V I, Saal J E, Issa A, Zhou B, Zeng X and Wolverton C 2018 Acta Mater. 158 65–78
[42] Maier S, Denis S, Adam S, Crivello J C, Joubert J M and Alleno E 2016 Acta Mater 121 126–36
[43] Jiang C, Besser M F, Sordelet D J and Gleeson B 2005 Acta Mater 53 2101–9