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Physics-based model to predict yield strength of single-phase FCC high-entropy alloys over wide temperature range

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Abstract: A physics-based temperature-dependent yield strength model without fitting parameters was developed for single-phase FCC high-entropy alloys. The model considered the temperature dependence of lattice friction stress, solid solution strengthening, grain boundary strengthening, dislocation strengthening, and their evolution with temperature to the overall yield strength. The results show that a quantitative relationship between temperature, material parameters, and yield strength was successfully captured by the model. This model can predict the yield strength at different temperatures only by using the easily available material parameters at room temperature. The accuracy of model was well verified by 17 sets of available experimental data over a wide temperature range (4.2−1273 K). Moreover, the contribution of different strengthening mechanisms to the yield strength was quantitatively analyzed and discussed from 4.2 to 1273 K, and some suggestions for improving the temperature-dependent yield strength were put forward.

Key words: single-phase FCC high-entropy alloys; temperature-dependent yield strength; strengthening mechanism; theoretical model

1 Introduction

High-entropy alloys (HEAs), named by YEH et al [1] have attracted wide interest from researchers in recent years due to their excellent physical, mechanical, and other properties [2−6]. Some high-entropy alloys, represented by single-phase face-centered cubic (FCC) high-entropy alloys, exhibit good strength and ductility in extreme environments, especially at extremely low temperatures [7−9]. These alloys may be excellent candidates for applications in extreme low-temperature conditions. For example, the magnets of the ITER fusion reactor become superconducting when cooled down to 4 K [10]. Yield strength, as the core indicator of mechanical properties, is indispensable for the performance evaluation and strengthening-toughening design of high-entropy alloys. Therefore, it is essential to investigate the yield strength of high-entropy alloys as a potential structural material under the influence of temperature (especially low temperature).

Relevant temperature-dependent mechanical properties studies have been carried out from the experimental side [10−13]. For example, the work from RACKWITZ et al [12] on CrCoNi alloys showed that grain size affects yield strength and fatigue crack extension at both room temperature and low temperature (77 K). NAEEM et al [10,13] studied the mechanical properties of single-phase FCC high-entropy alloys (CrMnFeCoNi and

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CrFeCoNi) at ultralow temperatures (the lowest temperature reaches 15 K) by using in situ neutron diffraction and demonstrated the interaction of multiple deformation mechanisms in high-entropy alloys at 15 K. In addition, the study showed that Peierls stress significantly increased at low temperatures, and the contribution of grain boundary strengthening and dislocation strengthening to the yield strength also needs to be considered.

Due to equipment limitations, the deformation behavior of materials at ultralow temperatures is still a largely unexplored area so far [13]. In fact, it is not only difficult to carry out experiments at ultralow temperatures but also time-consuming and costly. This has prompted the consideration using theoretical methods for the yield strength estimation [2,14−18]. WU et al [2] did a pioneering study. Their work showed that the lattice friction seemed to be the main factor affecting the temperature-dependent yield strength. Thus, they ignored most of the strengthening mechanisms and established a model. VARVENNE et al [15] established a solute strengthening model. This model considers the dependence of temperature and rate, and there are no fitting parameters. But these parameters input required by the model (including solute/stacking fault interactions in the random alloy; distribution of misfit strain tensors, etc) is difficult to measure [17]. In addition, for the large error of prediction at low temperatures, VARVENNE et al [15] also pointed out that it is necessary to determine the linear tension coefficient more accurately. Models with parameters determined by regression have also been developed [19,20].

In general, previous experimental and theoretical work has greatly improved the understanding of the mechanical behavior of high-entropy alloys under the influence of temperature [2,10−13,15−21]. But, the current theoretical studies focus more on probing the microscopic deformation mechanisms of materials at different temperatures through molecular dynamics [22], first principles [23], etc [8]. Less theoretical work has been done on the quantitative effect of temperature on the yield strength of high-entropy alloys, although a few temperature-dependent yield strength models have been reported [2,15,19,20]. However, there is a lack of models that can unify temperature, physical parameters, and yield strength. In particular, there is an absence of theoretical work that can be used to easily and accurately predict the yield strength of high-entropy alloys at ultralow temperatures. This has somewhat hindered the assessment of the serviceability and engineering applications of this alloy [24]. In addition, existing techniques and tools are mostly dedicated to the discovery of new alloy compositions with good properties but are unable to identify their mechanical properties at different temperatures. Considering the huge potential applications of high-entropy alloys at low temperatures, there is a great need to develop temperature-dependent yield strength theoretical models, especially for predicting the yield strength at ultralow temperatures.

In the present study, a temperature-dependent yield strength theoretical model was developed for single-phase FCC high-entropy alloys. The model considers the contribution of lattice friction stress, solid solution strengthening, grain boundary strengthening, dislocation strengthening, and their evolution with temperature as a contribution to the overall yield strength. The model requires only a few material parameters at room temperature to predict the yield strength at different temperatures. A good validation of the model was obtained with 17 sets of experimental data at different temperatures (from 4.2 to 1273 K).

2 Theoretical derivation

2.1 Theoretical background

The research on the room temperature strengthening mechanism of high-entropy alloys is relatively abundant. For single-phase FCC high-entropy alloy, it was found that the strengthening mechanisms include lattice friction, grain boundary strengthening, solid solution strengthening, and dislocation strengthening. Due to the large number of elements composing high-entropy alloys, differences in the atomic sizes of different elements lead to lattice warping, resulting in lattice distortion [17]. The ability of lattice distortion to impede the motion of dislocations and thus bring about a dramatic effect on the mechanical properties of the material. Therefore, the concept of solute and solvent in conventional alloys is no longer applicable in high-entropy alloys [2]. There is a rich body of work on

conventional strengthening theory. If it is possible to verify the applicability of the traditional strengthening theory to high-entropy alloys by considering its temperature dependence, there is no need to build a new theory suitable for high-entropy alloys from scratch. This will greatly save the time and effort of scholars and thus speed up the process of alloy development and application. Therefore, considering the temperature dependence of the conventional strengthening model and its evolution with temperature is the next focus.

2.2 Temperature-dependent strengthening mechanisms

2.2.1 Lattice friction stress and solid solution strengthening

For conventional solid solution strengthened alloys, many studies have been conducted and theoretical models have been developed. However, different from conventional solid solution strengthened alloys, high-entropy alloys have unique structures and properties. To address this situation, WU et al [2] concluded that the solid solution strengthening term can be subsumed into the lattice friction term after studying a variety of equiatomic high-entropy alloys. The new expression for the lattice friction term obtained by WU et al [2] is

$$\sigma'_{\mathrm{fr}}(T)=\frac{2G(T_{\mathrm{R}})}{1-\upsilon(T_{\mathrm{R}})}\cdot\exp\left[-2\pi\left(1+\frac{T}{T_{\mathrm{m}}}\right)\right] \tag{1}$$

where σ'_{fr} is the lattice friction stress, $G(T_{\mathrm{R}})$ is the shear modulus at room temperature. $\upsilon(T_{\mathrm{R}})$ is the Poisson's ratio at room temperature, and T_{m} is the melting temperature of the material. It is noticed that the shear modulus and Poisson's ratio are temperature-dependent. Therefore, we can rewrite Eq. (1) in the following form:

$$\sigma'_{\mathrm{fr}}(T)=\frac{2G(T)}{1-\upsilon(T)}\cdot\exp\left[-2\pi\left(1+\frac{T}{T_{\mathrm{m}}}\right)\right] \tag{2}$$

2.2.2 Temperature-dependent grain boundary strengthening

In recent decades, scholars in related fields have been using the classical Hall−Petch relationship to consider the role of grain boundary strengthening. The Hall−Petch relationship is expressed as follows:

$$\Delta\sigma_{\mathrm{gb}}=kd^{-1/2} \tag{3}$$

where $\Delta\sigma_{\mathrm{gb}}$ is the contribution of grain boundary strengthening to yield strength, k is the Hall−Petch coefficient, and d is the grain size of the material. However, relying on the above model for grain boundary strengthening calculations, experiments need to be carried out to obtain the Hall−Petch coefficients at different temperatures, which makes it difficult to detach the model from high (or low) temperature experiments to achieve prediction.

It is worth noting that after years of development, many scholars have modified the above model. Therefore, there exist many variants of grain boundary strengthening on the same basic model. CORDERO et al [25] summarized many variants of these models and gave a form of the Hall−Petch coefficient model with the following expression:

$$k=\beta Gb^{1/2} \tag{4}$$

where β is a constant, G is the shear modulus of the material, and b is the magnitude of the Burgers vector. Since the Burgers vector varies very little, its temperature dependence is not considered in the current work. Therefore, by using k and G at the reference temperature T_0 (Room temperature is used in the present work), it can be obtained

$$\beta b^{1/2}=\frac{k(T_0)}{G(T_0)} \tag{5}$$

Combining Eqs. (3) and (5), the temperature-dependent grain boundary strengthening model can be derived as

$$\Delta\sigma_{\mathrm{gb}}(T)=\frac{k(T_0)}{G(T_0)}\cdot G(T)d^{-1/2} \tag{6}$$

This grain strengthening model only depends on the shear modulus at different temperatures and the grain size. Hall−Petch coefficient and shear modulus can be obtained from experiments at room temperature.

2.2.3 Temperature-dependent dislocation strengthening

Plastic deformation is caused by the movement of movable dislocations. Higher dislocation density usually resulted in higher yield strength. Dislocations also exist in single-phase FCC high-entropy alloys and should be considered. For dislocation strengthening, scholars usually use the following equation [10]:

$$\Delta\sigma_{\mathrm{dis}}=M\lambda b\rho^{1/2}G \tag{7}$$

where $\Delta\sigma_{\mathrm{dis}}$ is the contribution of dislocation strengthening to yield strength; M is the Taylor

factor, which has a value of 2.73 for BCC structures and 3.06 for FCC structures [3]; λ is a constant whose value depends on the Poisson's ratio and the arrangement and orientation of dislocations [26]; ρ is the dislocation density.

Considering the temperature dependence of the shear modulus and ignoring the change of dislocation density with temperature, Eq. (7) is extended to be temperature dependent, which yields

$$\Delta\sigma_{\mathrm{dis}}(T)=M\lambda b\rho^{1/2}\cdot G(T) \tag{8}$$

It can be found that in order to enable the prediction of the yield strength at different temperatures, the acquisition of the temperature-dependent shear modulus is a critical step.

2.2.4 Temperature-dependent shear modulus

In the study of temperature-dependent shear modulus models, LAPLANCHE et al [27] used the expression proposed by VARSHNI [28] to regress experimental data for CoCrFeMnNi alloys between 200 and 1000 K. In our past work [29], for metallic bulk materials, a temperature-dependent shear modulus model without fitting parameters has been established. In light of the fact that this model has been well validated by experimental results for a variety of materials. Therefore, it was decided to use this model in the present work. It has the following expression:

$$G(T)=\frac{1+\upsilon(T_0)}{1+\upsilon(T)}\cdot\frac{\left(1+\int_0^{T_0}\alpha(T)\mathrm{d}T\right)^3}{\left(1+\int_0^{T}\alpha(T)\mathrm{d}T\right)^3}\cdot\left(1-\frac{\int_{T_0}^{T}C_{\mathrm{V}}(T)\mathrm{d}T}{\int_{T_0}^{T_{\mathrm{m}}}C_{\mathrm{V}}(T)\mathrm{d}T+\Delta H_{\mathrm{M}}}\right)^{1/2}\cdot G(T_0) \tag{9}$$

where $C_{\mathrm{V}}(T)$ is the temperature-dependent constant molar heat capacity; ΔH_{M} is the molar enthalpy of melting; T_0 is the arbitrary reference temperature; $\alpha(T)$ is the temperature-dependent thermal expansion coefficient; $\upsilon(T)$ and $\upsilon(T_0)$ are the Poisson's ratio at temperature T and arbitrary reference temperature T_0, respectively.

For high-entropy alloys, the shear modulus is approximately zero at the melting point temperature, so the heat of melting enthalpy can be ignored here. Thus, the temperature term in Eq. (9) can be simplified. Finally, a modified temperature-dependent shear modulus model can be obtained:

$$G(T)=\frac{1+\upsilon(T_0)}{1+\upsilon(T)}\cdot\frac{\left(1+\int_0^{T_0}\alpha(T)\mathrm{d}T\right)^3}{\left(1+\int_0^{T}\alpha(T)\mathrm{d}T\right)^3}\cdot\left(1-\frac{\int_{T_0}^{T}C_{\mathrm{V}}(T)\mathrm{d}T}{\int_{T_0}^{T_{\mathrm{m}}}C_{\mathrm{V}}(T)\mathrm{d}T}\right)^{1/2}\cdot G(T_0) \tag{10}$$

2.3 Temperature-dependent yield strength model

The yield strength of conventional alloys is usually considered to be composed of independent reinforcements. The overall yield strength is usually expressed as a linear combination of the contributions of several strengthening mechanisms at room temperature, which are approximated to be essentially interaction-free. The current study shows that this still applies to the yield strength of high-entropy alloys at room temperature [3,10,30]. In this study, it is assumed that the summation approach still holds at different temperatures. Therefore, the overall contribution of various temperature-dependent strengthening mechanisms to yield strength can be expressed as

$$\sigma_{\mathrm{y}}(T)=\sigma'_{\mathrm{fr}}(T)+\Delta\sigma_{\mathrm{gb}}(T)+\Delta\sigma_{\mathrm{dis}}(T) \tag{11}$$

Thus, combining Eqs. (8), (6), and (2),

$$\sigma_{\mathrm{y}}(T)=\frac{2G(T)}{1-\upsilon(T)}\cdot\exp\left[-2\pi\left(1+\frac{T}{T_{\mathrm{m}}}\right)\right]+\frac{k(T_0)}{G(T_0)}\cdot G(T)d^{-1/2}+M\lambda b\cdot G(T)\rho^{1/2} \tag{12}$$

Further, combining Eqs. (10) and (12), the temperature-dependent yield strength model for single-phase FCC high-entropy alloys is established.

$$\sigma_{\mathrm{y}}(T)=\left[\frac{2}{1-\upsilon(T)}\cdot\exp\left[-2\pi\left(1+\frac{T}{T_{\mathrm{m}}}\right)\right]+\frac{k(T_0)}{G(T_0)}\cdot d^{-1/2}+M\lambda b\cdot\rho^{1/2}\right]\cdot\left[\frac{1+\upsilon(T_0)}{1+\upsilon(T)}\cdot\frac{\left(1+\int_0^{T_0}\alpha(T)\mathrm{d}T\right)^3}{\left(1+\int_0^{T}\alpha(T)\mathrm{d}T\right)^3}\cdot\left(1-\frac{\int_{T_0}^{T}C_{\mathrm{V}}(T)\mathrm{d}T}{\int_{T_0}^{T_{\mathrm{m}}}C_{\mathrm{V}}(T)\mathrm{d}T}\right)^{1/2}\cdot G(T_0)\right] \tag{13}$$

The proposed temperature-dependent theoretical model, Eq. (13), provides a clear understanding of the quantitative relationship between temperature, material parameters (including dislocation density, grain size, etc), and yield strength. The model can predict the yield strength at different temperatures when only some basic physical parameters of the material itself and experimental data at room temperature are required. Therefore, the application of this theoretical model does not need to rely on a large number of difficult experiments, and can easily obtain the yield strength of high-entropy alloys at different temperatures, especially at ultralow temperatures.

3 Experimental verification of theoretical model

3.1 Determination of parameters in model prediction

In this section, the model predicted results were compared with the experimental data. In the predictions, all data involved in the calculations were presented. These required parameters can be found or derived from the available literature. Multiple groups of experimental data on high-entropy alloys reported in different published articles were covered in this work. These experimental results are reported by different scholars, so there will be some differences in the yield strength data. For the sake of full compliance with the original scientific intentions of the authors in the cited literature, the nomenclature of all alloys in this paper has been retained in their original form in the respective cited literature. If data on the parameters at room temperature were already given in the corresponding literature, the data already given by the authors in the corresponding literature were used in preference. Moreover, the work of the same author reported in different literature was used as much as possible. Finally, only reports by different authors of the same material will be cited.

According to previous studies, the coefficients of thermal expansion and Poisson's ratio vary somewhat with temperature, but the magnitude of the variation has a small effect on the results of shear modulus. In addition, the coefficients of thermal expansion and Poisson's ratio at different temperatures of high-entropy alloys are less reported so far, especially the data at low temperatures. Therefore, their temperature dependence is not considered in the calculation for the time being. At the same time, based on previous research, heat energy can be replaced by atomic kinetic energy and potential energy [31−33]. Therefore, the temperature term in the shear modulus model can be simplified to $\left(1-\frac{T-T_0}{T_m-T_0}\right)^{1/2}$ when using the model.

3.2 Validation of model with different materials

Based on the developed temperature-dependent yield strength theoretical model, the yield strengths of a total of 17 groups of high-entropy alloys were calculated over a wide range of temperatures. All the parameters used in the prediction are given in Table 1. For convenience,

Table 1 Parameters for prediction

Material	T_m/K	$G(T_0)$/ GPa	$\upsilon(T_0)$	$b(T)$/ nm	$k(T_0)$/ (MPa·μm$^{0.5}$)	d/ μm	ρ/m^{-2}	λ	M
AM-CoCrFeNiMn	1613 [3]	72.7 [3]	0.3 [3]	0.26 [3]	677 [3]	75[3]	4.25×10^{14} [3]	0.33 [3]	3.06 [3]
CoCrFeNiMn	1553 [2]	80 [2]	0.26 [2]	0.26 [3]	494 [34], 400 [21] (solidified and annealed),	6 [11], 9 [34], 8 [35], 5 [13], 50 [21], 350 [21]	–	–	–
CoCrFeNi	1695 [2]	84 [2]	0.28 [2]	0.25 [10]	276 [10]	5 [10]	1.89×10^{13} [10]	0.2 [10]	3.06 [10]
$Al_{0.1}$CoCrFeNi	1723 [7]	79 [7, 36]	0.28 [2]	0.25 [10]	–	> 1 mm [7]	–	0.2 [10]	3.06 [10]
CoCrNi	1690 [2]	87 [2]	0.3 [2]	–	673 [38]	7 [12], 16 [37], 68 [12]	–	–	–
CrFeNi	1664 [40]	69 [41]	0.3 [41]	–	966 [39]	160[39]	-	-	–

the reference temperature in the calculation is uniformly adopted as room temperature. The temperature T is used in the prediction. The average grain size has also been shown.

3.2.1 CoCrFeNiMn and CoCrFeNiMnV_x high-entropy alloys

Figures 1−4 present the results of comparing model predictions with experimental data for CoCrFeNiMn high-entropy alloys. AM-CoCrFeNiMn refers to alloys made by additive manufacturing. Figure 4 shows the comparison results between experimental data and model predictions for the CoCrFeNiMnV_x high-entropy alloy, which is based on the addition of a small amount of V to CoCrFeNiMn. Past studies [21] have shown that the structure of this alloy remains single-phase FCC when x is less than 0.5. Therefore, the basic parameters of CoCrFeNiMn (solidified and annealed) were used to predict the yield strength of CoCrFeNiMnV_x. The average grain sizes of solidified and annealed alloys are 120 and 130 μm [21], respectively.

3.2.2 CoCrFeNi and $Al_{0.1}$CoCrFeNi high-entropy alloys

Comparative results of model predictions and experiments for CoCrFeNi and $Al_{0.1}$CoCrFeNi high-entropy alloys are illustrated in Fig. 5. $Al_{0.1}$CoCrFeNi alloy is added with Al element based on CoCrFeNi. Because the amount of added aluminum element is relatively small, the alloy is

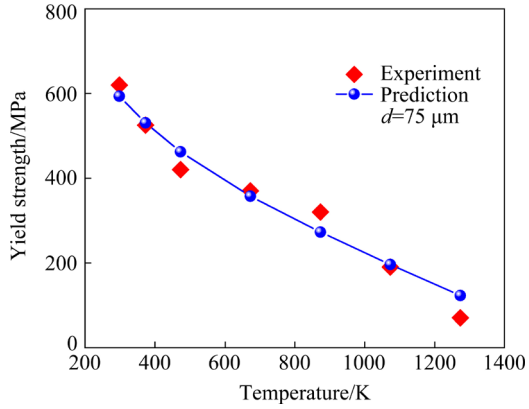

Fig. 1 Comparison of experimental data with model predictions for AM-CoCrFeNiMn alloys

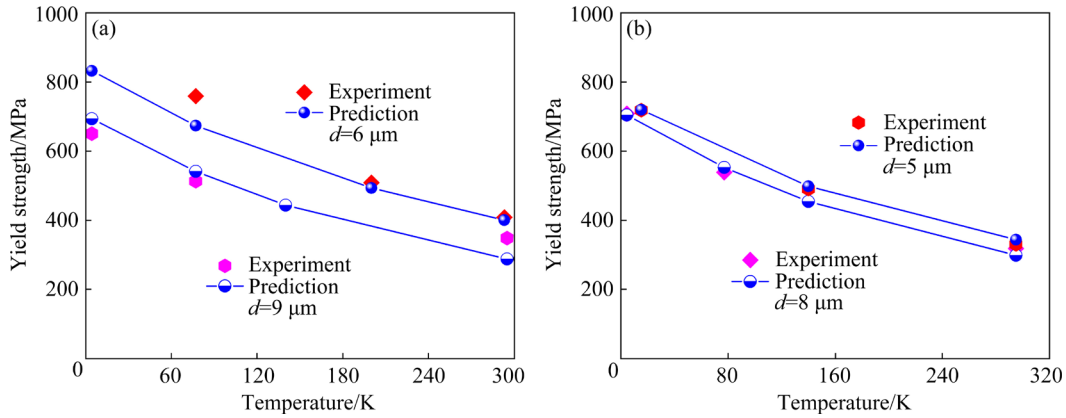

Fig. 2 Comparison of experimental data with model predictions for CoCrFeNiMn alloys

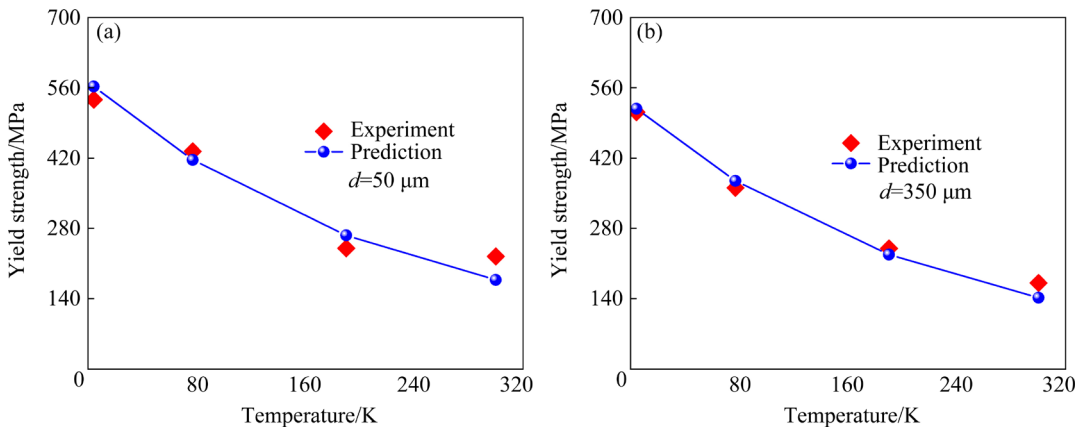

Fig. 3 Comparison of experiment data with model predictions for as-solidified (a) and as-annealed (b) CoCrFeNiMn alloys

still a single phase. Although the authors have explicitly stated that initial dislocations were observed, they did not give the corresponding values [7]. Therefore, we deduced the dislocation density by using the data at room temperature from the article. The results show that the deduced dislocation density (1.87×10^{14} m^{-2}) is in the same order of magnitude as that observed in other experiments. In addition, grain boundary strengthening was not considered because of the large grain size (>1 mm) of $Al_{0.1}$CoCrFeNi [7].

3.2.3 CoCrNi and CrFeNi alloys

Figure 6 provides the comparison between model predictions and experimental results for the medium-entropy alloys CoCrNi and CrFeNi. It is clear from the figures that the model predictions are in good agreement with the experimental data over a wide range of temperatures.

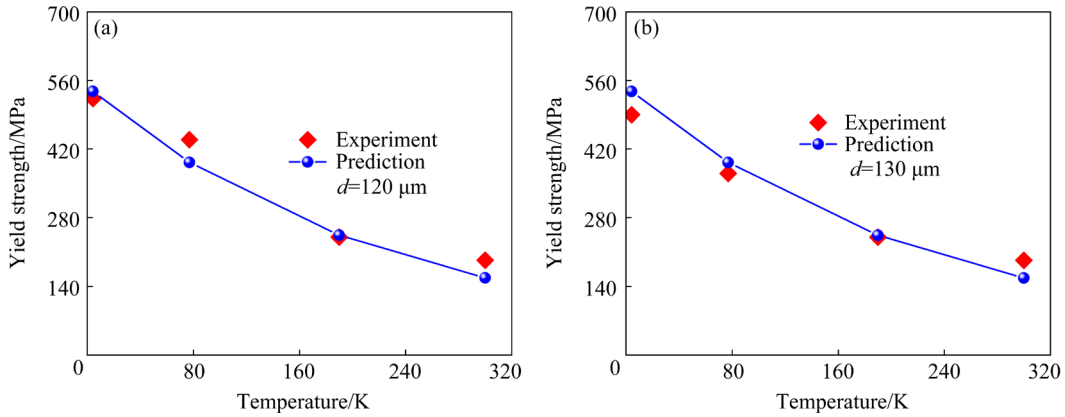

Fig. 4 Comparison of experimental data with model predictions for as-solidified (a) and as-annealed (b) $CoCrFeNiMnV_{0.25}$ alloys

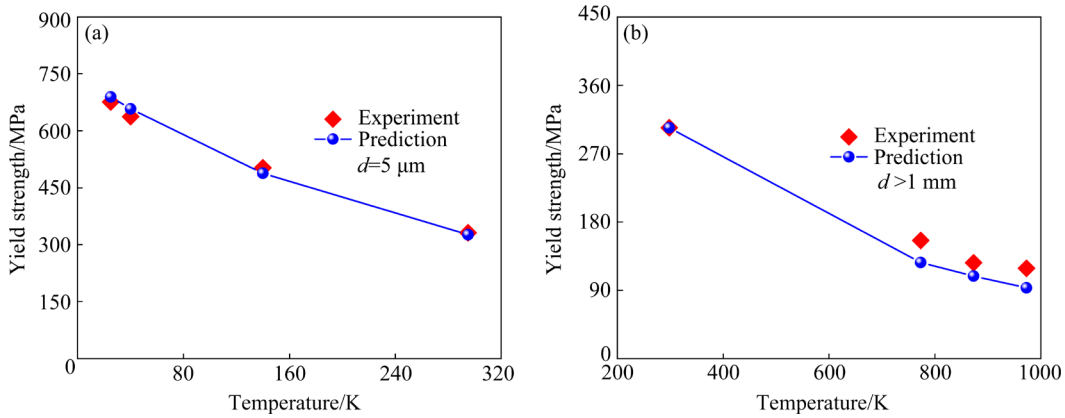

Fig. 5 Comparison of experimental data with model predictions for CoCrFeNi (a) and $Al_{0.1}$CoCrFeNi (b) alloys

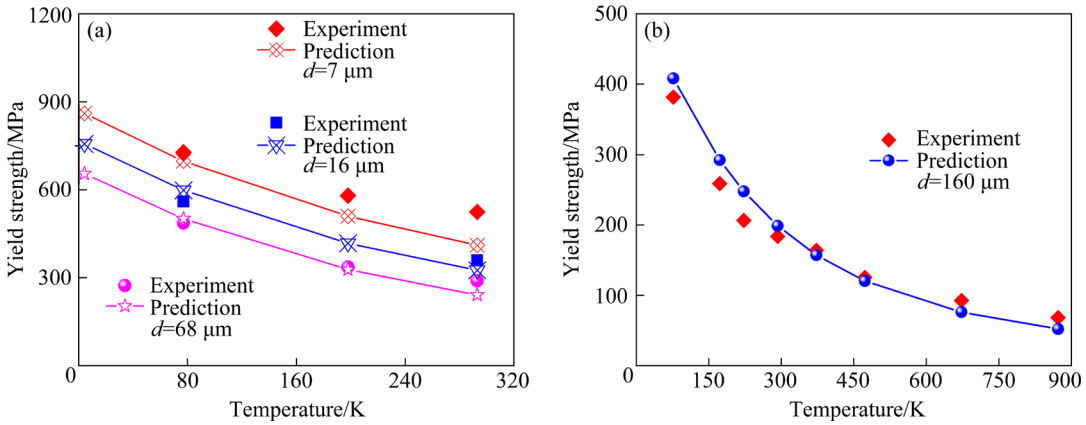

Fig. 6 Comparison of experimental data and model predictions for CoCrNi (a) and CrFeNi (b) alloys

3.2.4 Non-equiatomic CrFeNiV and CoCrNi alloys

The k value of $V_{20}Cr_{15}Fe_{20}Ni_{45}$ at room temperature is not found in the reports so far, so it is obtained by inverse extrapolation from other parameters. The derived k value is 879 MPa·μm$^{0.5}$. The shear modulus and Poisson's ratio adopt the parameters of CrFeNi alloy. The melting point of $Cr_{15}Fe_{20}Ni_{45}V_{20}$ is about 1543 K, and the average grain size is about 13.2 μm [42]. The composition of $Cr_{30.7}Co_{34.7}Ni_{34.6}$ is similar to that of equiatomic CoCrNi, so the parameters related to equiatomic CoCrNi are adopted. The average grain size is about 30 μm [43]. In addition, the effect of dislocation strengthening was not considered since no dislocations were experimentally observed (see Fig. 7).

4 Discussion

4.1 Quantitative analysis of strengthening mechanism

The quantitative analysis and discussion of each strengthening mechanism at different temperatures can help us to further understand the temperature-dependent yield strength in high-entropy alloy. With the CoCrFeNiMn as an example, Figs. 8 and 9 show the absolute value and contribution of each mechanism to the overall yield strength of the high-entropy alloy at different temperatures. The case shown in Fig. 8 is from LI et al [3] in a temperature range of 298−1273 K. Figure 9 is from the work of PU et al [35] in a temperature range of 4.2−293 K. The difference is that the high-entropy alloy shown in Fig. 8 has initial dislocations and the high-entropy alloy in Fig. 9 has no dislocations. The grain sizes in Figs. 8 and 9 are 75 and 5 μm, respectively. It can be observed that all the strengthening mechanisms are temperature-dependent, although each mechanism has a slightly different sensitivity to the change in temperature.

As can be seen in Fig. 8(a), the strength contributed by several strengthening mechanisms decreases with increasing temperature. The lattice friction stress decreases rapidly, and the contribution of lattice friction to yield strength also

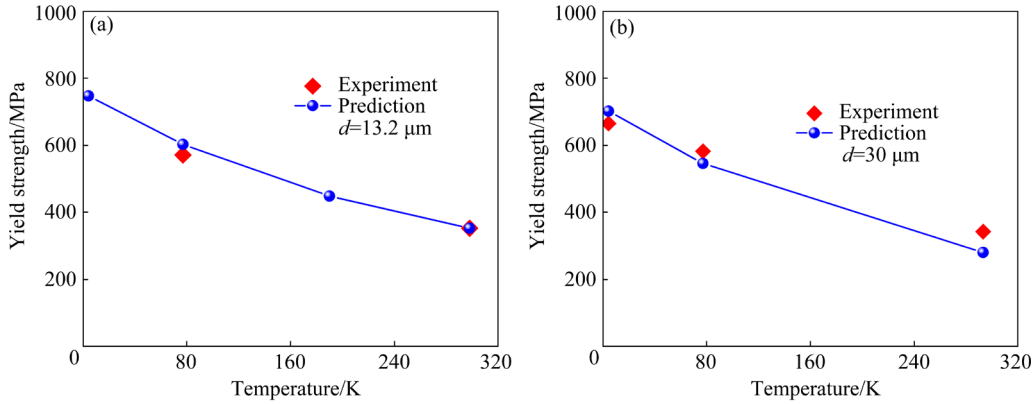

Fig. 7 Comparison of experimental data with model predictions for non-equiatomic CrFeNiV (a) and CoCrNi (b) alloys

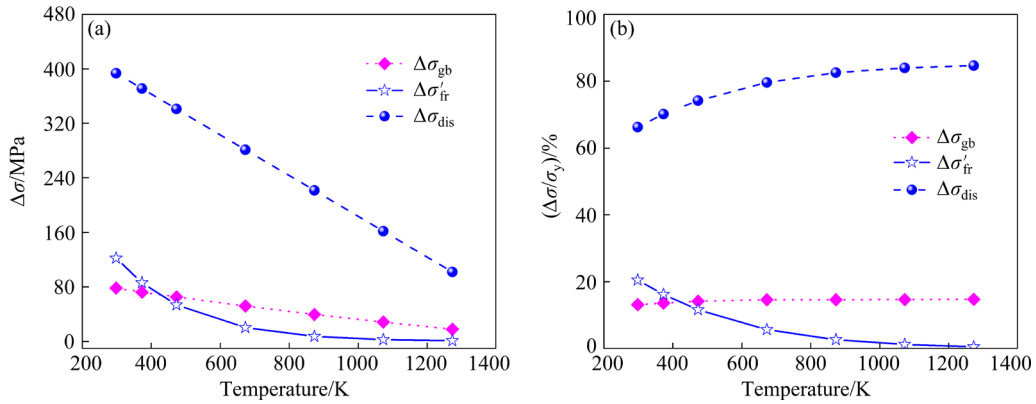

Fig. 8 Absolute value (a) and contribution (b) of each mechanism to yield strength of CoCrFeNiMn alloys at different temperatures [3]

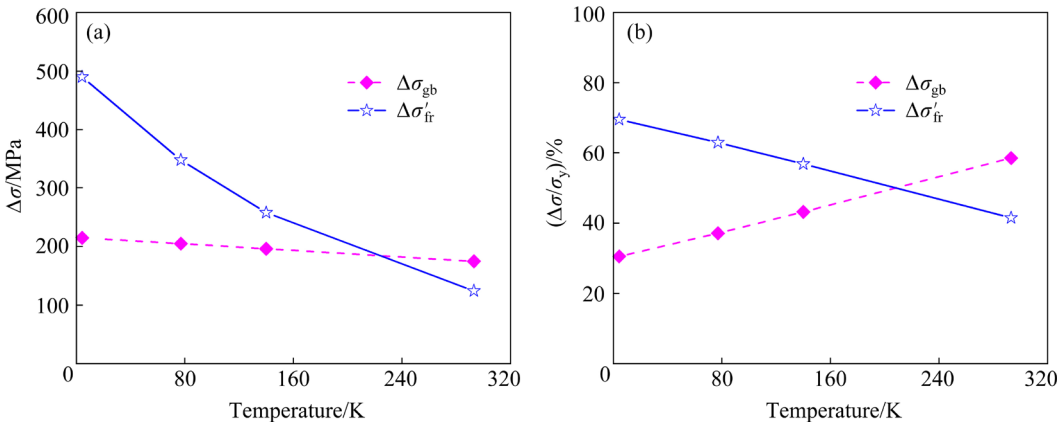

Fig. 9 Absolute value (a) and contribution (b) of each mechanism to yield strength of CoCrFeNiMn at different temperatures [35]

decreases gradually. Dislocation strengthening has a significant effect on the yield strength at different temperatures. As the temperature increases, the contribution of dislocation strengthening to yield strength also increases gradually, as shown in Fig. 8(b). The contribution of dislocation strengthening to yield strength is about 66% at room temperature and about 85% at high temperature (1273 K). In addition, grain boundary strengthening changes slowly, the proportion of grain boundary strengthening is relatively stable and changes little.

Grain boundary strengthening is a well-known strengthening mechanism and has been confirmed to be applicable for high-entropy alloys [44]. As shown in Fig. 9, the contribution of grain boundary strengthening to the yield strength at room temperature is significant. In the absence of dislocations, the contribution to the yield strength reaches nearly 70%. According to Fig. 9, it can be found that the absolute amount of grain boundary strengthening varies less with temperature, but the contribution to yield strength decreases with decreasing temperature. This is because the lattice friction stress has a large variation with temperature, resulting in a significant increase in its contribution to the yield strength with decreasing temperature. In particular, at ultralow temperature (4.2 K), the yield strength contribution is close to 70%. Such results are consistent with the report of NAEEM et al [10].

Combining Figs. 8 and 9, it can be concluded that grain boundary strengthening is an effective way to enhance the yield strength of high-entropy alloys at room temperature and can remain stable at different temperatures. Dislocation strengthening can significantly improve the yield strength at different temperatures and the variation with temperature is relatively obvious. This indicates that the introduction of initial dislocations is an effective way to enhance the strength of the alloy at different temperatures. Also, increasing the lattice friction is quite effective for strength enhancement below room temperature. Considering the promising application of high-entropy alloy at low temperatures, the optimization of the process to increase the lattice friction stress and introduce dislocations is expected to further improve the yield strength of the high-entropy alloy at very low temperatures.

4.2 Determining *k*

The literature research revealed that there are some differences in the reported values of k by different scholars. For the determination of parameter k, the following convention was used in our calculation. First, if the authors have given or cited the corresponding parameters in their article, the value that has been given or cited by that author was used. As mentioned in Section 3.1, this is to comply with the original scientific intent of the original authors. Secondly, if the article reporting the experimental data did not have the corresponding values, the reported data that would predict the strength at room temperature more accurately were selected or relied on other data for inverse extrapolation. Currently, back extrapolation has been performed in two cases, and the values obtained are in the reasonable range.

4.3 Influence of shear modulus on yield strength

The shear modulus is often used to characterize the ability of materials to resist shear strain. From Eq. (12), it is clear that the temperature-dependent shear modulus has a strong positive effect on the yield strength. We also note that other academic studies have reported similar results. For example, in recent studies on high-entropy alloys, scholars have found that the shear modulus of the alloy is proportional to the yield strength [15,45]. LAPLANCHE et al [45] pointed out that the temperature-dependent shear modulus acts as a significant factor in determining its yield strength. And similar results were found in previous studies of dilute and concentrated binary alloys by FLEISCHER [46]. This indicates that increasing the shear modulus to some extent helps to improve the yield strength. This provides an avenue for materials that require enhanced yield strength at low temperatures.

4.4 Advantages and implications of proposed model

Firstly, different from the most common approaches to modeling the temperature-dependent properties of materials, this work does not rely on regression on experimental data. This model is built without fitting experimental data over the entire temperature range. The derivation of the model has a clear derivation process and the parameters have a clear physical meaning. Secondly, the model provides a clear understanding of the quantitative relationship among temperature, material microstructural parameters (including dislocation density, grain size, etc), and yield strength. According to the model, the quantitative effects of different strengthening mechanisms or parameters on the yield strength can be easily analyzed. Thirdly, the structure of the model is relatively uncomplicated. The use of the model has few restrictions and constraints and has strong universality. Compared to the difficult and expensive low-temperature experiments, using this model to predict the yield strength at different temperatures can be fast and inexpensive. When the melting point temperature is known (which can be obtained during the preparation of the material), the model only requires a few material parameters at room temperature to predict the temperature-dependent yield strength. These parameters can be obtained relatively easily and the application of the model does not depend on a large number of difficult-to-conduct experiments. A reliable physical model can be constructed to accurately predict the properties of high-entropy alloys at low and high temperatures, which can extend the limited alloy performance data from room temperature experiments. Once the physical parameters of the material at room temperature are determined, the model can be used to quickly calculate its yield strength at possible service temperatures. From this point of view, the proposed model can also effectively accelerate the development of high-performance alloys and help to address the challenge of high-throughput technology in discovering new materials. Furthermore, in terms of prediction effectiveness, the validation of the model from experimental data shows that the model has a high prediction accuracy. In particular, the model predictions still achieved good agreement with experimental results at very low temperatures (4.2 K). The proposed model achieves an accurate prediction of the yield strength of high-entropy alloys at ultra-low temperatures at the least cost. In addition, this work shows that the theory applicable to conventional alloys at room temperature can be used for the study of temperature-dependent properties of high-entropy alloys with reasonable consideration of the corresponding mechanisms. The research results of this work would contribute to future research and optimization of the strength of single-phase FCC high-entropy alloys and facilitate their engineering applications as structural materials.

The present work focuses only on the temperature dependence of the yield strength of single-phase FCC high-entropy alloys. On the basis of the existing theoretical work, a temperature-dependent yield strength model was developed by considering the temperature dependence of the different strengthening mechanisms and the main influencing parameters. The model was well validated by experimental data. This suggests that the model applicable to conventional alloys at room temperature can be applied to the prediction of yield strength of high-entropy alloys at different temperatures with reasonable consideration of temperature effects. This provides enlightenment for future research on modeling the temperature-dependent mechanical properties of other high-

entropy alloys such as multiphase high-entropy alloys and refractory high-entropy alloys.

4.5 Other issues

Some parameters that are not very sensitive to temperatures, such as the coefficient of thermal expansion, its temperature dependence can be ignored in the calculation. Other parameters, such as grain size, dislocation density, shear modulus, and Hall-Petch coefficient, have a great influence on the prediction of strength. These parameters need to be measured or calculated accurately to predict the yield strength at different temperatures more accurately. Therefore, this should be noted when using the model.

When the temperature is lower than room temperature, the literature reports show that twins and twin boundaries can improve the yield strength of high-entropy alloys to a certain extent. In addition, due to the interaction between dislocation and twin, the strength and ductility can be improved at the same time. The current work has not considered the quantitative effect of twinning. From the results of the validation, this way of consideration is also feasible. Definitely, twin deformation is also an important mechanism. Therefore, it is necessary to establish a corresponding model to quantitatively consider its influence in future research.

5 Conclusions

(1) A temperature-dependent yield strength model with clear physical parameters (including dislocation density, grain size, etc) was developed for single-phase FCC high-entropy alloys. The model systematically considers the contribution of lattice friction stress, solid solution strengthening, grain boundary strengthening, dislocation strengthening, and their evolution with temperature to the overall yield strength.

(2) Without considering dislocations, the contribution of lattice friction to the yield strength was the largest at low temperatures, but the lattice friction stress decreased rapidly with increasing temperature starting from room temperature. At the same time, dislocation strengthening showed a significant improvement in yield strength at different temperatures. Therefore, the optimization of the process to increase the lattice friction stress and introduce dislocations is expected to further improve the yield strength of the high-entropy alloy at very low temperatures.

(3) The model was verified by 17 sets of available experimental data in the temperature range of 4.2−1273 K. With a known melting point temperature, this model requires only a few material parameters at room temperature to predict the yield strength at different temperatures. The use of the model could avoid the inconvenient ultra-low temperature experiments.

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预测单相 FCC 高熵合金在宽温度范围内屈服强度的物理模型

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摘 要：针对单相 FCC 高熵合金，开发一个基于物理背景的温度相关性屈服强度模型，该模型无拟合参数。模型考虑晶格摩擦应力、固溶强化、晶界强化、位错强化的温度相关性及其随温度的演化对合金整体屈服强度的影响。结果表明，模型成功地捕获温度、材料参数和屈服强度之间的定量关系。仅通过使用在室温下容易获得的参数就可预测不同温度下合金的屈服强度。在宽温度范围(4.2~1273 K)内，可获取的 17 组实验数据验证了模型的准确性。此外，还定量分析和讨论 4.2~1273 K 范围内不同强化机制对屈服强度的贡献，提出提高温度相关性屈服强度的建议。

关键词：单相面心立方高熵合金；温度相关性屈服强度；强化机理；理论模型

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