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Tuning the defects in face centered cubic high entropy alloy via temperature-dependent stacking fault energy

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ABSTRACT

Extreme-low (even negative) and strong temperature-dependent stacking fault energy (SFE) is one of the most unique properties in face centered cubic (FCC) high entropy alloys (HEAs). Here, by making full use of this unique property, we present a proof-of-principle investigation of tuning defects in FCC HEAs through changing SFE during deformation. A qualitative model is proposed to predict the possibilities of different types of defects in FCC HEAs. Following this model, different defects combinations, instead of individual defects, are well controlled by rolling. FCC HEAs with balanced dislocation, stacking faults and twins show good balance between strength and ductility.

Defects play very important role in the performance of metallic materials [1]. The increasing dislocation density leads to increase of strength but sharp loss of ductility [2]. Twin boundaries and phase boundaries strengthen alloys without severe ductility sacrifice through blocking dislocation motions [3, 4]. Grain boundaries also significantly affect the mechanical properties through Hall-Petch relationship [5]. Researchers have proposed lots of relevant strategies, such as dislocation engineering [2, 3, 6], twining introduced plasticity effect and grain boundary engineering [7, 8], to get strong and ductile metallic materials. These strategies bring out good comprehensive mechanical properties in some model metals or alloys.

Changing the stacking fault energy (SFE) through micro-alloying is an efficient method to adjust the defects of alloys during deformation. This method is most widely used in twining induced plasticity (TWIP) steel [9]. Recently, face centered cubic (FCC) high entropy alloys (HEAs) attracted increasing attentions [10] and showed intriguing mechanical, physical and functional properties [11–13]. One of the interesting intrinsic properties is their strong temperature-dependent SFE [10, 11, 14]. The SFE of FCC HEAs is very low and changes dramatically with changing temperature [15–17]. The effects of temperature on the deformation defects have also been identified in FCC HEAs [18–22], however, how the SFE affects the deformation defects is still unclear. Uncovering the intrinsic relation between deformation defects and SFE not only helps to explain the deformation mechanism, but provides a new method to tune the type of defects as well.

Inspired by the unique temperature-dependent SFE of HEA and important influence of SFE on defects controlling, we proposed a SFE-dependent model for the formation of defects in FCC HEAs. Following this qualitative model, the defects in a $CoCrFeNiNb_{0.1}$ HEA are well tuned. The HEAs with well-tuned dislocations, stacking faults and twins showed excellent balance between strength and ductility.

To start with, a SFE-dependent qualitative model is developed to predict the defects evolution of HEAs during deformation. In FCC crystal structure, slip usually occurs between close-packed {111} atomic planes, as sketched in Fig. 1(a). One layer is represented by spheres, A, the second identical layer rests in the sites marked in B and the third takes the position C. Consider the glide of a perfect dislocation with Burgers vector $\mathbf{b_1} = \frac{1}{2}<110>$. It will be energetically more favorable for the B_1 atoms to move to B_2 via the C_1 positions for the migration of dislocation. This implies that the dislocation passes as two partial dislocations, one immediately after the other as $\mathbf{b_1} \rightarrow \mathbf{b_2} + \mathbf{b_3}$ or $\frac{1}{2}<110> \rightarrow \frac{1}{6}<211> + \frac{1}{6}<12\bar{1}>$, as shown in Fig. 1(a). The energy state of this process is sketched in Fig. 1(b) and the energy barriers of $\mathbf{b_2}$ and $\mathbf{b_3}$ are noted as ΔE_1 and ΔE_3. The dislocation has to overcome ΔE_1 and ΔE_3 in its migration of a Burgers vector distance ($\mathbf{b_1}$). However, stacking faults will show up if the B atoms finish the first step ($\mathbf{b_2}$) and stop at position C

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(can not finish the second step by $\mathbf{b_3}$). Accordingly, the appearance of stacking faults is determined by the migration of a partial dislocation ($\mathbf{b_3}$).

Let's further analyze the migration of $\mathbf{b_3}$ in Fig. 1(a). The dislocation moves at a critical shear stress, which is called as Peierls-Nabarro (P-N) stress. Suppose that the P-N stress has been applied and the dislocation has finished $\mathbf{b_2}$ and then stopped. This process results in a stacking fault in the FCC matrix. The work done by the stress is $\Delta E_{P-N} = \Delta E_1 = \int l\tau d\frac{1}{2}b_2$, where the l is the length of dislocation, τ is the P-N stress. The surface energy caused by the appearance of stacking fault is $\Delta E_2 = \int \gamma ds$, where γ is the stacking fault energy per unit area. Then the energy barrier of $\mathbf{b_3}$ (ΔE_3) can be calculated by $\Delta E_3 = \Delta E_1 - \Delta E_2$, as shown in Fig. 1(b). The P-N stress for dislocation migration is usually calculated by $\tau = \frac{2G}{(1-\upsilon)}\exp(\frac{-2\pi\omega}{b})$, where G is the shear modulus, υ is passion ratio and ω is the width of the dislocation. By correlating the G with temperature (T) [23, 24], we get the P-N energy curve via temperature, sketchily shown by curve 1 in Fig. 1(c). For the SFE, since it has been demonstrated that the CoCrFeNi HEA has a low stacking fault energy and the stacking fault energy of the CoCrFeNiMn decreases with decreasing temperature [16, 17], we sketchily show it by curve 2 in Fig. 1(c). The different energy states for dislocation migration at three different temperatures can be given in Fig. 1(b) by using different dashed lines. At high temperatures, taking C_I for example, the stacking fault energy is positive and thus the energy barrier of $\mathbf{b_3}$ is smaller than that of $\mathbf{b_2}$ ($\Delta E_2 > 0$, $\Delta E_1 > \Delta E_3$). Accordingly, the dislocation moves though $\mathbf{b_3}$ under the P-N stress. The similar thing happens when the stacking fault energy decreases to 0 J/m^2 (C_{II} position in Fig. 1(b), (c)). Above this critical temperature (C_{II}), the stacking fault is unstable and consequently dislocations are observed after deformation. However, below this temperature, taking C_{III} for instance, the stacking fault energy is negative and thus the energy barrier of $\mathbf{b_3}$ is larger than the P-N energy ($\Delta E_2 < 0$, $\Delta E_{P-N} < \Delta E_3$), as shown in Fig. 1(b). The P-N stress is not able to complete the process of $\mathbf{b_3}$ and thus the deformation results in numerous stacking faults. Based on this model, one can predict that deformation would mainly cause dislocations at high temperature while different possibilities at low temperatures. The stacking faults will show up when the stress is just equal to P-N stress. With the increase of stress, the dislocations will also occur when the energy barrier of ΔE_3 can be overcome.

To identify the prediction of the proposed model, a HEA was rolled at different temperatures and then characterized by transmission electron microscope (TEM). The HEA with a nominal chemical composition of $CoCrFeNiNb_{0.1}$ is prepared by induction melting and casting in an argon atmosphere. The raw materials are of high-purity elements (≥99.95%) and ultrasonically cleaned for 5 min before melting. The cast samples are solid-solution heat treated at 1200 °C for 2 h with water quenching to get single FCC phase. The solution treated $CoCrFeNiNb_{0.1}$ HEAs are rolled at liquid nitrogen temperature with 10%, 25% and 50% thickness reduction (noted as CTR10%, CTR25% and CTR50%). As a comparison, some samples are also rolled at room temperature with 25% thickness reduction (noted as RTR25%). The microstructures of the rolled HEAs are analyzed by transmission electron microscope (TEM, JEOL 2100F). The tensile samples with the gauge dimension of 25 mm × 1.2 mm × 3 mm are directly cut from this solid solution treated and rolled samples and tested on a Material Testing System (MTS, Alliance RT30) tension machine at ambient temperature with an engineering strain rate of 1×10^{-3} s^{-1}.

Panels (a)–(c) in Fig. 2 are the representative TME images showing stacking faults in the CTR10% sample. The bright field (BF) image and the corresponding diffraction pattern (DP) inset in Fig. 2(a) shows that the dark contrast is caused by defects. Fig. 2(b) further proves that there are thick defects in the matrix by weak-beak dark field (DF) image. The high resolution TEM (HRTEM) image and Fast Fourier transformation (FFT) inset in Fig. 2(c) clearly shows that the defect is stacking fault.

More interestingly, not only stacking faults occurred, but nano-twins showed up in the cryogenically rolled HEAs when thickness reduction increased. Fig. 3(a) shows the BF image of CTR25% and corresponding

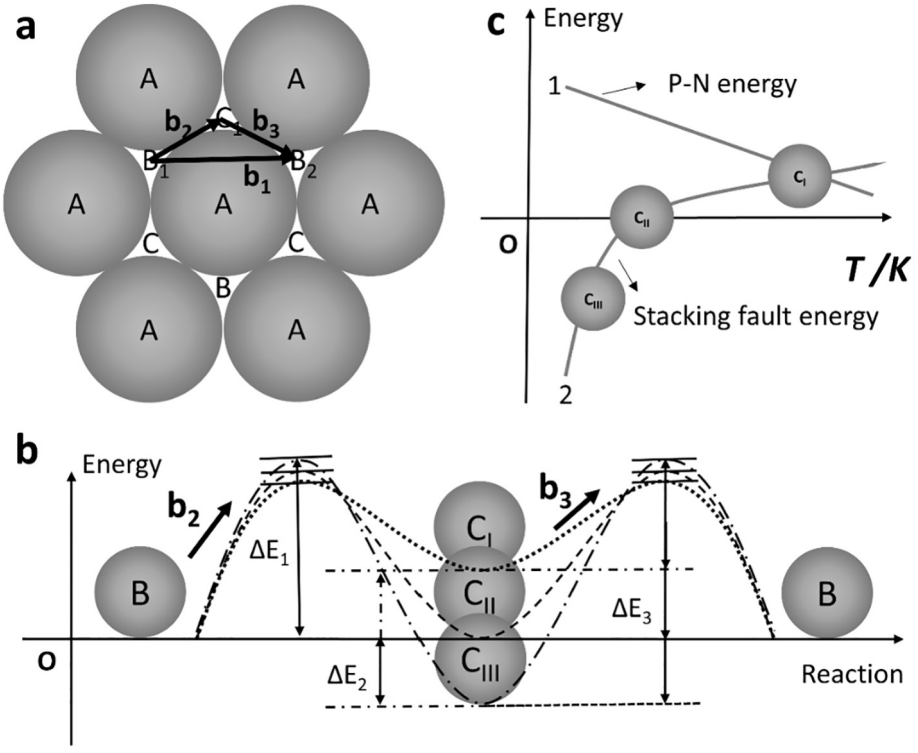

Fig.1. (a) Sketch of slip of {111} planes in FCC crystal structure; (b) Sketch of energy barrier that a dislocation should overcome during movement and (c) Sketch of P-N energy and stacking fault energy via temperature. At high temperatures (above C_{II}), the P-N energy is smaller than the energy barrier of $\mathbf{b_3}$ and the stacking fault is unstable and deformation tends to mainly results in dislocations in the matrix. The stacking fault becomes stable when the temperature is low and the energy barrier of $\mathbf{b_3}$ is larger than the P-N energy barrier (below C_{II}) and deforming during this temperate range causes lots of stacking faults and twins in the matrix.