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Stacking fault energy of face-centered-cubic high entropy alloys

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ABSTRACT

The stacking fault energy (SFE) values of several typical face-centered-cubic (fcc) high-entropy alloys (HEAs) were experimentally measured by weak-beam dark-field transmission electron microscopy. It was found that the SFE of the Fe-Co-Ni-Cr-Mn HEA system strongly depends on the SFE of the individual constituents. Specifically, the SFE of this HEA system is closely associated with the Ni concentration in the alloys. Additionally, the lower SFE tends to promote formation of more deformation twins with a smaller thickness under loading, leading to better mechanical properties, especially at low temperatures.

1. Introduction

Recently, high-entropy alloys (HEAs) consisting of multiple principle elements in equal or near equal atomic ratio have attracted extensive attention because of their interesting structural and mechanical properties [1–5]. Surprisingly, these multi-principal-element alloys tend to form simple crystalline structures, instead of multiple phases or intermetallic compounds. For example, FeCoNiCrMn is a single phase alloy with a face-centered cubic (fcc) lattice. It was reported [6] that FeCoNiCrMn has excellent fracture toughness even at cryogenic temperature of 77 K, and mechanical twins were found to be responsible for the outstanding low-temperature properties. As such, more and more scientific activities were recently focused on systematic and in-depth research on the stacking fault energy (SFE) of HEAs, particularly fcc HEAs, and aimed to further optimize their mechanical performance and reveal the related deformation mechanisms [7–12].

Theoretical SFE calculations of FeCoNiCrMn have been conducted by several different research groups; S. Huang et al. [11] reported that the SFE of FeCoNiCrMn is 21 mJ m^{-2} via ab initio calculations, whilst A.J. Zaddach et al. [12] determined the SFE for a series of Fe-Co-Ni-Cr-Mn alloys with different number of constituents (i.e., Ni, FeNi, FeNiCr, FeCoNiCr and FeCoNiCrMn) using both X-ray diffraction measurements and first-principles calculations. It was found that the SFE decreases with the increase in the number of components, i.e. configurational entropy. The SFE of quinary FeCoNiCrMn and quaternary FeCoNiCr lies in-between 20 and 25 mJ m^{-2}, and that of ternary FeNiCr is increased up to 60 mJ m^{-2}. However, experimental validation of these calculations in HEAs has rarely been reported, although it is not only important for validating the computation results, but also imperative for properly understanding mechanical behavior of HEAs with large configuration entropy, especially the low-temperature deformation mechanisms.

In order to uncover experimentally effects of elemental constituents on the SFE and the relationship between the SFE and mechanical properties in HEAs, NiCoCr, FeCoNiCr, FeCoNiCrMn, $(FeCoNiCr)_{94}Mn_6$, $(FeCoNiCr)_{86}Mn_{14}$ and $Fe_{20}Co_{15}Ni_{25}Cr_{20}Mn_{20}$ were selected. The approach using the weak-beam dark-field (WBDF) imaging technique proposed previously [13] was employed to analyze the partial dislocation pairs and determine the SFE in this work.

2. Experimental details

The selected alloys were produced by arc-melting the pure elements (purity > 99.98%) in a Ti-gettered high-purity Ar atmosphere. Each ingot was flipped and re-melted at least four times to ensure chemical homogeneity. The melted alloys were then cast into a copper mold with a dimension of 10 mm × 10 mm × 60 mm. The drop-cast alloys were subsequently homogenized at 1473 K for 10 h in Ar atmosphere, followed by water quenching. Then the ingots were cold-rolled to 65% thickness reduction and annealed at 800 °C for 1 h. The dog bone-shaped tensile specimens with a gauge length of 20 mm, a width of 5 mm and a thickness of 1.3 mm were cut from the sheet in the direction parallel to the rolling direction by electric discharging machining and polished to the 2000-grit SiC paper.

Shear modulus and Poisson's ratio of the as-cast alloys were measured by resonant ultrasound spectroscopy while lattice parameters of

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the alloys were determined by X-ray diffraction. The SFE measurements were conducted using a JEM-2100 TEM operated at 200 kV. The specimens were first strained under tension at a rate of 1×10^{-3} s^{-1} to the yield point. Disks of 3-mm diameter were then taken from the central part of these pre-tensioned specimens, mechanically polished to 50 μm thickness through SiC paper and then electron-polished by twin-jet technique using a mixed solution of $HClO_4$:C_2H_6O = 1:9. Dark field images of Shockley partial dislocations were observed by the method of WBDF with a beam direction near the [111] zone on the (111) defect habit plane using < -220 > -type g-vectors. At least four different dislocations were characterized for each alloy to measure the Shockley partial dislocation separations. In additional, tensile tests of all the alloys were conducted at the same strain rate of 1×10^{-3} s^{-1} at room temperature and liquid nitrogen temperature.

3. Results and discussion

The SFE of alloys can be measured by observing the sizes of extended dislocation nodes or width of partial dislocations using TEM. However, it was reported that the sizes of dislocation nodes are very sensitive to heat treatment, but the width between partial dislocations is not [14]. Fig. 1a–c show typical WBDF images of dissociated dislocations of three representative NiCoCr, FeCoNiCr and $Fe_{20}Co_{15}Ni_{25}Cr_{20}Mn_{20}$ HEAs on their (111) habit planes, respectively. As can be seen, the partial dislocation core separation of NiCoCr is much wider than that of FeCoNiCr and $Fe_{20}Co_{15}Ni_{25}Cr_{20}Mn_{20}$. The separation distance (d) and the angle (θ) between the dislocation and the Burgers vector of full dislocation of these three alloys are measured and plotted in Fig. 1d. Theoretical partial dislocation curves are fitted to the experimental data to determine the SFE based on the following equation [15]:

$$d = \frac{Gb_p^2}{8\pi\gamma}\cdot\frac{2-\nu}{1-\nu}\cdot\left(1-\frac{2\nu\cos 2\theta}{2-\nu}\right) \quad (1)$$

where G is the shear modulus, b_p is the $1/6a_0 < 112 >$ partial dislocation Burgers vector (a_0 is the lattice parameter determined by X-ray diffraction) and ν is the Poisson's ratio. Shear modulus and Poisson's ratio of the alloys were measured by resonant ultrasound spectroscopy. The measured data of FeCoNiCrMn, FeCoNiCr and NiCoCr are similar to those reported in literature [16]. Table 1 lists the shear modulus, Poisson's ratio, lattice parameter and SFE of all the investigated alloys. The experimentally obtained SFE of FeCoNiCrMn and NiCoCr is 26.5 ± 4.5 and 18 ± 4 mJ m^{-2}, respectively, which is similar to that reported by George et al. [17,18] (i.e., 30 ± 5 mJ m^{-2} and 22 ± 4 mJ m^{-2}, respectively) using the same WBDF method, verifying the reliability of our measurements.

As can be seen from Table 1, the SFE value of the $(FeCoNiCr)_{94}Mn_6$ and $(FeCoNiCr)_{86}Mn_{14}$ alloys is similar to that of FeCoNiCrMn and FeCoNiCr. It seems that addition of Mn has inappreciable influence on the SFE of the Fe-Co-Ni-Cr-Mn alloy system. Nevertheless, it was confirmed that the SFE of Fe-Mn-(Al-Si) steel increases with the increase of Mn [19], indicating that even the same element has different impact on the SFE in different alloy systems, which may be related to different electronic, volumetric and magnetic effects [20]. For the particular quinary Fe-Co-Ni-Cr-Mn alloy system, however, we found that Ni plays a dominant role in the SFE, as shown in Fig. 2. The higher the Ni content, the larger the SFE, which could be related to the large SFE of Ni (γ_{Ni} = 125 mJ m^{-2} [21]). Replacing the constituents having low SFE (e.g., Co, γ_{Co} = 27 mJ m^{-2} [22]) with those having high SFE tends to increase the SFE of the resultant alloy. For example, substitution of 5% Co with Ni in FeCoNiCrMn (i.e., the $Fe_{20}Co_{15}Ni_{25}Cr_{20}Mn_{20}$ HEA) increases the SFE from 26.5 ± 4.5 to 38 ± 6 mJ m^{-2}. Based on these observations, it is clear that the SFE value of individual elements in the

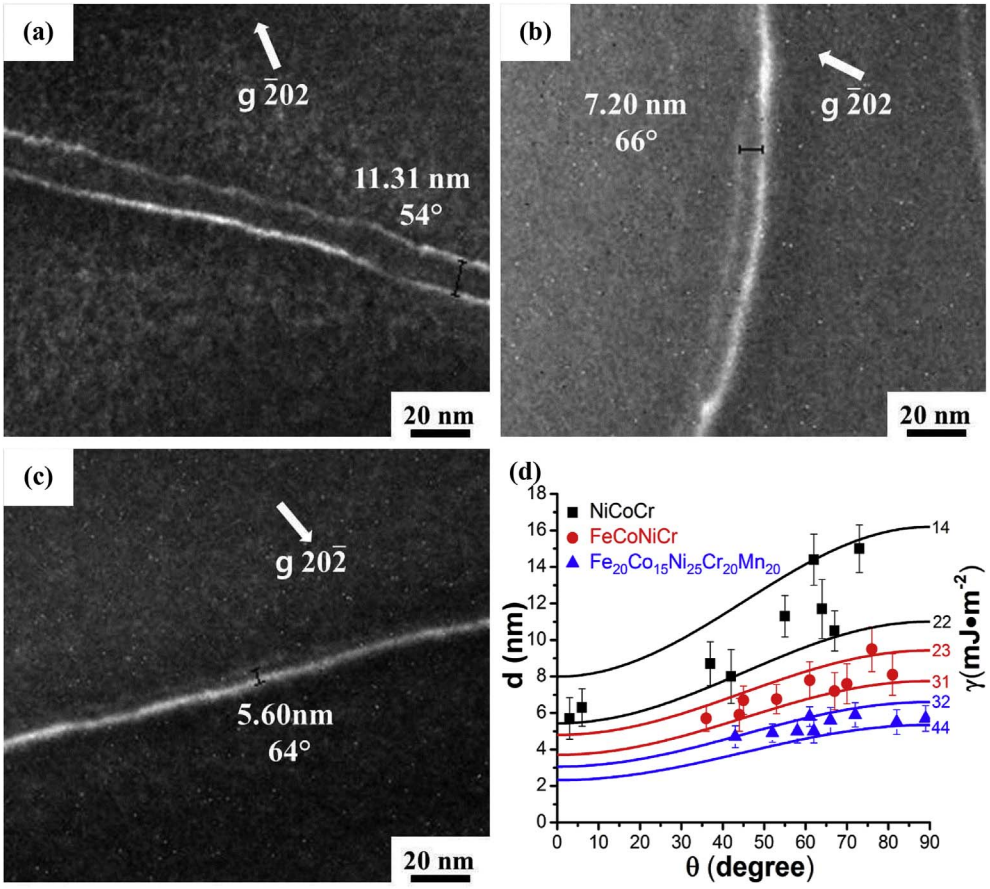

Fig. 1. The WBDF images of dissociated dislocations of NiCoCr (a), FeCoNiCr (b) and $Fe_{20}Co_{15}Ni_{25}Cr_{20}Mn_{20}$ (c), and (d) Dissociation width of partial dislocations as a function of the angle between the dislocation line and the total Burgers vector.