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Mechanical behavior and solid solution strengthening model for face-centered cubic single crystalline and polycrystalline high-entropy alloys

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ABSTRACT

In the present work, a solid solution strengthening effect in high-entropy alloys (HEAs) was studied by investigating mechanical characteristics of single crystalline CoCrFeMnNi HEA and a corresponding model was developed. (100) and (110) oriented single crystals of the CoCrFeMnNi alloy were grown and their single crystallinity was identified using X-ray diffraction (XRD), energy dispersive spectroscopy (EDS), and electron backscatter diffraction (EBSD) analyses. The mechanical testing of the single crystalline CoCrFeMnNi alloy was performed and the critical resolved shear stress (CRSS) was obtained. A solid solution strengthening modeling based on the lattice friction stress and an intrinsic residual strain of HEAs was performed. The solid solution strengthening effect of HEAs was verified using the model proposed.

1. Introduction

High-entropy alloys (HEAs) are one of the most promising classes of novel materials that have recently been a subject of extensive research [1–3]. They contain five or more principal elements in equal or near equal atomic percentage (on the at% basis) with a simple single-phase face-centered cubic (FCC), body-centered cubic (BCC), or hexagonal close-packed (HCP) structure [4–6]. Specifically, an FCC CoCrFeMnNi alloy exhibits an excellent combination of strength and ductility at cryogenic temperatures [7]. Due to the promising properties of the CoCrFeMnNi alloy, its mechanical properties and deformation behavior were investigated in previous studies [8–12]. Single phase HEAs form simple and stable solid solutions without precipitates [13], therefore, the strengthening mechanism operating in these alloys can easily be singled out and identified. However, this seemingly simple problem poses some challenges, because HEAs have been known to exhibit severe lattice distortions caused by atomic size misfit [14]: The attendant intrinsic lattice resistance to dislocation glide in HEAs is so high that the solid solution strengthening effect plays an important role in the yield strength of the alloy [15]. However, a recent study suggests that there are no significant deviations of the position of atoms from the ideal lattice sites and no clear evidence that the local lattice strain is anomalously large in HEAs [16].

The solid solution strengthening effect in HEAs was investigated using mechanical studies of single crystalline HEAs [15,17–19]. The observed increased yield stresses in single crystals CoCrFeNi [15] and CoCrFeMnNi [17,18] alloys were associated with solid solution strengthening [15]. However, the previous experimental attempts to describe the solid solution strengthening effect in HEAs did not account for the contribution of the lattice distortion to the strengthening of the alloys. Toda-Caraballo and Rivera-Dı´az-del-Castillo [20] proposed a solid solution strengthening model for HEAs by extending Labusch's [21] approach for binary solid solutions. Their model was developed based on the lattice distortion of HEAs. While the crystallographic orientation, which should have an effect on the yield strength of the polycrystalline materials, was not considered, the model provided a partial prediction of the experimentally observed yield strength [20].

Zhao and Nieh [22] argued that the lattice distortion of Ni-based equiatomic alloys is proportional to the lattice friction stress. They associated the lattice distortion of HEAs with the lattice constant mismatch between HEAs and Ni [22], but this approximation is restricted to a relative comparison between HEAs and Ni, rather than accounting for the degree of the lattice distortion quantitatively. In contrast, Ye et al. [23] proposed a geometric model for intrinsic residual strain in HEAs. In this model, the atomic size, atomic fraction, and packing density of elements with different atomic sizes were considered and the

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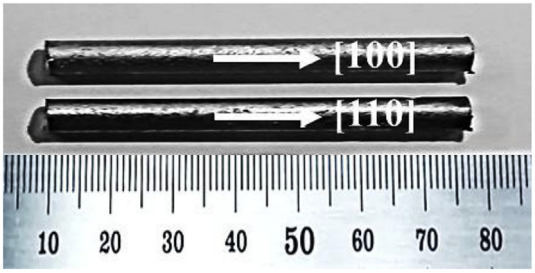

Fig. 1. CoCrFeMnNi single crystal rods fabricated using Bridgman furnace with directions of [100] and [110].

induced residual strain in HEAs was obtained on that basis [23]. Based on their model, phase stability with respect to the calculated residual strain was predicted.

In the present work, we have chosen CoCrFeMnNi alloy as a testbed material. The mechanical behavior of single crystalline CoCrFeMnNi alloy was studied and the critical resolved shear stress (CRSS) of the alloy was measured. A solid solution strengthening model for estimating intrinsic yield strength of HEAs was developed using the residual strain in the lattice and the CRSS.

2. Experimental procedure

Single crystals of the CoCrFeMnNi alloy were grown in a Bridgman furnace. The grown single crystalline CoCrFeMnNi rods 5 mm in diameter are shown in Fig. 1. The growth directions of the single crystals were [100] and [110]. Polycrystalline CoCrFeMnNi alloy was prepared from casting ingots. The ingots were fabricated using vacuum induction melting of the pure elements (purity above 99.9%) inside a graphite mold. They were annealed at 1100 °C for 6 h in an argon atmosphere, followed by cold-rolling to reduce thickness from 7 to 3.5 mm. The cold-rolled plate was annealed at 800 °C for 1 h in an argon atmosphere.

The orientation of the crystals was examined by X-ray diffraction (XRD) and electron backscatter diffraction (EBSD) analyses. The surfaces of the samples for the XRD measurement were first polished using 600, 800, and 1200 SiC grit papers, then fine polished using 1 μm diamond powders. The XRD measurement was conducted using a Rigaku D/MAX-2500 XRD equipment with the incident beam of Cu Kα radiation (wavelength = 1.5418 Å). The scans were performed from 40 to 100° of 2θ with a step size of 0.02° and scan speed of 1°/min. The samples for EBSD were polished by up to 1 μm diamond powders and then final polishing was carried out using colloidal silica suspensions. The EBSD was performed using a Philips XL30S microscope with a field emission gun at 25 kV. In addition, the chemical composition of the single crystals and polycrystalline alloy was characterized using a scanning electron microscope-energy dispersive spectroscopy (SEM-EDS).

Compression testing for both the single crystals and polycrystalline alloy was conducted with a strain of $10^{-3}\,s^{-1}$ at room temperature. Cylindrical samples with a diameter of 2 mm and a height of 4 mm were used for compression tests using an R&B 302 micro load universal testing machine (UTM). In parallel, digital image correlation (DIC) analysis was performed to identify the slip planes and the slip directions of the single crystals.

3. Theoretical modeling

Yield strength is composed of the 'intrinsic' lattice friction stress (σ_{fr}) and the other various microstructural contributions, such as those due to the solute atoms ($\Delta\sigma_{ss}$), initial dislocation density ($\Delta\sigma_{\rho i}$), precipitates ($\Delta\sigma_{ppt}$), and/or grain boundaries ($\Delta\sigma_{gb}$). To a first approximation, the yield strength can be expressed as the sum of these individual contributions [24]:

$$\sigma_y(T,\ \dot{\varepsilon}) = \sigma_{fr} + \Delta\sigma_{ss} + \Delta\sigma_{\rho i} + \Delta\sigma_{ppt} + \Delta\sigma_{gb}. \quad (1)$$

Each of these contributions is strain rate and temperature dependent, and so is their sum. In this article, the effects of testing temperature and strain rate will be disregarded, however. Only room temperature yield strength for a 'quasi-static' strain rate ($10^{-2}\,s^{-1} \sim 10^{-4}\,s^{-1}$) are considered. In a carefully grown single crystal the initial dislocation density is low, and no grain boundaries are present. Hence, the contributions of the initial dislocation density ($\Delta\sigma_{\rho i}$) and grain boundaries ($\Delta\sigma_{gb}$) can be neglected. Also, the contribution of precipitates can be excluded because a single phase CoCrFeMnNi alloy has no precipitates in its initial microstructure. Therefore, we focus on the first and second terms (σ_{fr} and $\Delta\sigma_{ss}$) on the right-hand side of Eq. (1) and include the solid solution strengthening term ($\Delta\sigma_{ss}$) into the 'intrinsic' lattice friction stress (σ_{fr}). That is, the lattice friction stress (σ_0) includes the strengthening effect due to the lattice distortion:

$$\sigma_y = \sigma_{fr} + \Delta\sigma_{ss} = \sigma_0. \quad (2)$$

The intrinsic yield strength (lattice friction stress, σ_0) of alloys is attributable to the atomic size misfit and modulus misfit [20,25,26]. In this work, we studied the effect of the atomic size misfit effect only. The stress σ_0 was normalized by the elastic modulus, E.

For alloys for which no information on the elastic moduli is available in the literature, the elastic moduli were calculated using a linear rule of mixtures:

$$E = \sum_i^n X_i \cdot E_i, \quad (3)$$

where X_i and E_i are the atomic fraction and elastic modulus of i -th constituent element, respectively, and n is their number. It is noted that HEAs contain various principal elements (i.e., no distinction between solvent and solute atoms can be made), which results in a lattice distortion. It hinders the movement of dislocations and leads to an increase in yield strength. In order to quantify the lattice distortion, we adopted the geometric model proposed by Ye et al. [23].

We calculated the root mean square (RMS) residual strain, which is induced by the lattice distortion, and analyzed the relationship between the residual strain and intrinsic yield strength. The lattice friction stress was estimated both experimentally and theoretically. In the experimental approach, the CRSS was calculated as the lattice friction stress from the mechanical testing data for single crystals. In the theoretical approach, the lattice friction stress was expressed as a function of the residual strain calculated by the geometric model. In this way, an equation for predicting the lattice friction stress was established by deriving a relation between the CRSS and the residual strain.

Among the constituent elements of CoCrFeMnNi alloy, Ni has the smallest atomic radius [27]. Also, it is known that Cr and Mn atoms behave as if they had large atomic radii [28,29]. Therefore, the Seitz radius was used to account for the effect of constituent elements: the atomic radii of Co, Cr, Fe, Mn, and Ni were taken to be 1.385, 1.423, 1.411 1.428, and 1.377 Å, respectively.

4. Results and discussion

4.1. X-ray diffraction and electron backscatter diffraction of single crystalline and polycrystalline CoCrFeMnNi alloy

Fig. 2(a) shows the XRD patterns of the single crystal (SC) and polycrystal (PC) CoCrFeMnNi alloys. The XRD patterns of SCs with [100] and [110] directions exhibit [200] and [220] crystallographic orientations, respectively, while those of PC show typical FCC diffraction patterns. Fig. 2(b and c) display EBSD pole figures of [100] and [110] SCs on their growth direction. A single crystal orientation was detected in each pole figure with the corresponding orientation. These confirmed the single crystallinity of the grown SCs and the fact that no precipitation occurred.