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Abstract

Multi-component alloys are emerging as promising metallic materials for cryogenic applications for their excellent combination of high ultimate tensile strength and good ductility. But their low yield strength can severely limit their applications. Lattice distortion is emerging as a feasible method in overcoming this dilemma. Here, we investigate the mechanical and microstructural responses of a high-strength ternary equiatomic medium entropy FeCrNi alloy at 293 K and 15 K using integrated theoretical simulation and experimental efforts centered around *in situ* neutron testing, first principal calculation, and dislocation-based strengthening models. At 293 K, the yield strength of the alloy is 651 ± 12 MPa, with total elongation of 0.48 ± 0.05 . At 15 K, the yield strength increased to 1092 ± 22 MPa, but the total elongation dropped to 0.18 ± 0.01 . The single-crystal elastic moduli and macroscopic moduli were determined by *in situ* neutron diffraction, compared with first-principles calculation. The strengthening contribution to the yield strength from the lattice distortion was calculated based on the Varenne-Luque-Curtine solute strengthening theory for multi-component alloys, which almost doubled from 316 MPa to 629 MPa when decreasing the deformation temperatures from 293 K to 15 K. Dislocation multiplication was found to be the dominant deformation mechanism at both temperatures, whereas no twinning neither phase transformation was observed during deformation according to the *in situ* neutron diffraction and post-mortem characterization. Accumulated strengthening effects from lattice friction, grain boundaries, and dislocations were calculated and compared with the measured flow stress at both temperatures. These findings reveal the significant strengthening effect of lattice distortion and dislocations, paving the way in designing new multi-component alloys with the superb mechanical performance of cryogenic applications.

Keywords:

medium entropy alloy, multi-component alloy, cryogenic temperature, neutron diffraction

1. Introduction

In the past decade, a revolutionary new metallurgy design strategy, multi-component alloys (MCAs), containing several equimolar or non-equimolar components (in the range of 5-35% at.), has been developed [1,2]. According to the mixing configurational entropy (ΔS_{mix}) of the alloy, this new alloy group can be categorized into high entropy alloys (HEAs, $\Delta S_{mix} \geq 1.5R$) and medium entropy alloys (MEAs, $1.5R \geq \Delta S_{mix} \geq 1.0R$), where R is the gas constant. The vast degrees of

compositional freedom endow the HEAs/MEAs with extensive opportunities to tailor their physical properties. Among the different group of MCAs, one typical group based on 3d transition elements (Cr, Mn, Fe, Co, Ni, V, and Cu) can form a single face-centered cubic (FCC) structure, showing great potential in achieving superior strength-ductility combination [3–8]. This type of MCAs is denoted as tMCA here, whose compositions include CrMnFeCoNi HEA [9], FeCrCoNi HEA [10], CrCoNi MEA [11], FeNiCo MEA [4] and other variations.

Recently, the intriguing mechanical performance of tMCAs under cryogenic temperatures has been revealed, such as excellent high fracture tolerance [5,11], fatigue-crack growth resistance [12], and excellent strength-ductility balance [8,13,14]. This makes them highly desirable in the rapid-growing cryogenic applications such as space industries, high-resolution detectors, fusion reactors, and medical diagnosis [8]. The application of tMCAs at cryogenic temperatures, however, can be severely limited since their yield strength (YS) is relatively low compared to the conventional structural alloys. Many studies show the YS of tMCAs is generally lower than 400 MPa at room temperature [15] and 500 MPa at cryogenic temperatures [4,16]. For example, the YS of a single-phase CoCrFeMnNi HEA is only 166 MPa at 293 K and 350 MPa at 77 K [16]. Therefore, several conventional strengthening strategies (such as precipitating hardening [17] and grain refinement [18]) were applied to overcome this dilemma via introducing extensive dislocations and interfaces.

As an inherent advantage of MCAs, severe lattice distortion (a wide fluctuation of the atomic bond distances) is emerging as a very promising method in enhancing the YS. Unlike traditional alloys, no matrix or host element could be defined in MCAs according to their near equal-ratio design conception. The severe lattice distortion thus originates from the randomly distributed constituent elements with varying atomic radii [19]. Each individual atom in MCAs experiences different stress fields created by its interaction with a set of different neighbor atoms. The role of lattice distortion in strengthening the alloys, however, is still under debate. Wu et al. [20] suggested that the large lattice distortion fluctuation can only provide weak Labusch-type pinning effects on dislocation motions. However, research has shown that enhancing the lattice distortion by adding extra vanadium can induce significant YS improvement (ranging from ~200 to ~600 MPa) in both FCC and body-centered cubic (BCC) HEAs [21]. The critical role of lattice distortion in strengthening was also confirmed by physically-based theories, which successfully predicted the YS of several MCAs by using solute misfit volumes as the core parameter [22,23]. These theories also indicated the growing strengthening effect of lattice distortion with decreasing temperature [4]. This sheds a light on achieving ultrahigh YS of MCAs by modulating the lattice distortion. However, studies of tMCAs mainly focused on the CrCoNi alloy at a high-temperature range (>293 K) [24,25]. The effect of lattice distortion on strengthening at cryogenic temperatures is largely unexplored.

Herein, to exploit the great potential of tMCAs in achieving high YS at extremely low temperatures and provide a comprehensive understanding of the strengthening mechanisms in tMCAs, we studied a new equiatomic ternary MEA (FeCrNi alloy), which naturally carries large lattice distortion and has been shown to achieve a high YS at room temperature [26]. The mechanical responses and corresponding microstructure evolution, such as lattice strain and dislocation density, were recorded by *in situ* neutron diffraction tensile testing at 293 and 15 K. Post-mortem microscopy observations were carried out on the fractured samples to characterize the microstructure features and confirm the strengthening mechanisms. The elastic moduli were predicted by the first-principles calculation and validated by the *in situ* neutron tensile testing results. This work reveals an in-depth micro-mechanical understanding of the high strength FeCrNi alloy, therefore, opening new avenues for designing MCAs in cryogenic applications.

2. Materials and Methods

2.1 Materials

Powder metallurgy was used to produce the FeCrNi MEA with a nominal composition of Fe_{33.3}Cr_{33.3}Ni_{33.3}. High purity (>99.99%) Fe, Cr, and Ni raw materials were melted in an induction vacuum furnace. The melted liquid was dropped through a ceramic cube and atomized by high purity Ar with a pressure of 4 MPa. The formed powder, with an average diameter of 50 μm, was then capsulated in a steel cylinder chamber (Φ50×150 mm). After degassing and preheating to 1200 °C for 1 h, the sample was subjected to hot extrusion immediately with an extrusion ratio of 7:1 and a velocity of ~10 mm/s. The extruded bars were then cooled down to room temperature in the air. The actual chemical composition of the sample was measured to be Fe_{33.7}Cr_{33.7}Ni_{32.5} (at.%) by inductively coupled plasma mass spectrometry (ICP-MS) [26].

2.2 *in situ* neutron diffraction

In situ time of flight neutron diffraction measurements during tensile tests were carried out at the beamline of ENGIN-X at ISIS, spallation neutron source, the Rutherford Appleton Laboratory, UK [27]. The schematic illustration of the TOF neutron diffractometers and strain scanner can be seen in our previous work [28]. Originally, a pulsed beam of neutrons with a wide energy range (incident beam) traveled through a 100K liquid methane moderator, and its horizontal and vertical angular divergence was then modified by two pairs of motorized slits (4×4 mm²). A vacuum chamber and a 50 kN hydraulic stress rig with a horizontal loading direction were mounted 45° to the incident beam. Behind the collimators (4 mm wide), two diffraction detector banks (radial and axial) were centered on a horizontal diffraction angle of ±90° to the incident beam to collect the diffraction signals from grain planes subjected to tensile and compressive load, respectively. Before the tests, instrument parameters (e.g., primary and secondary flight path distance) and instrumental peak broadening effects were determined by measuring a strain-free standard CeO₂ calibrant. Dog-bone tensile samples were mounted on the stress rig then the high vacuum and low-temperature conditions were stabilized for half an hour before the test. Diffraction patterns were collected for 20 mins intervals between each loading step, iterating until fracture. Stress-control and displacement control were used at the elastic and plastic stages, respectively. The *in situ* neutron diffraction and tensile testing were repeated on two specimens for both temperatures. The data collected at the same condition is very similar, thus the reproducibility was confirmed and only one of the data was analyzed. Rietveld refinement and single peak fitting (with pseudo-Voigt function) were performed with the GSAS software, allowing the determination of lattice parameters, peak position, and full width at half maximum (FWHM) of the peaks. The lattice strain is defined as the change of inter-planar spacing with respect to its original inter-planar spacing. Its evolution can be calculated by [6]:

$$\varepsilon_{hkl} = \frac{d_{hkl} - d_{hkl}^0}{d_{hkl}^0} \quad (1)$$

, where ε_{hkl} is the lattice strain of $\{hkl\}$ grain family, d_{hkl} and d_{hkl}^0 is corresponding lattice spacing at the current stress state and stress-free state, respectively. Procedures for single crystal constant and dislocation density calculations were included in the Supplementary Materials.

2.3 First principal calculation

Density Functional Theory (DFT) for elastic constant calculations were performed within the Vienna Ab-initio Simulation Package (VASP) using the Projector Augmented Wave (PAW) method and spin-polarized electronic structure scheme [29,30]. The electron exchange correlation functional was in the Generalized Gradient Approximation (GGA) treated with Perdew-Burke-Ernzerhof parametrization [31]. All the calculations in this work were carried out within the PAW

potentials for Cr, Fe, and Ni without semi-core electrons with the core configurations [Ar]3d⁴s¹, [Ar]3d⁷s¹, and [Ar]3d⁹s¹, respectively. The plane wave cut-off energy for the most of calculations was 400 eV. The total energy was converged to 10⁻⁶ eV/cell and the force components were relaxed to 10⁻³ eV/Å. Total energies used for elastic constant calculations were performed using the Monkhorst-Pack meshes [32] with 4×4×4 k-point for both 3×3×3 FCC-supercell configurations with 108 atoms per unit cell configurations and additional calculations with the 6×6×6 k-point meshes were also performed for checking the convergence. A more detailed description of elastic constants from first-principles DFT calculations in different intermetallic phases can be found in Refs. [33–38].

For disordered alloys, conventional approaches for evaluating elastic constants from DFT techniques are usually based on so-called Coherent Potential Approximation (CPA) from which a single site mean field theory is applied to treat completely random configurations with different chemical compositions. The CPA method has been employed to investigate elastic property maps from DFT calculations for the case of concentrated random FCC Fe-Cr-Ni alloys which are the main base for austenitic stainless steels [39,40]. In the present study, an alternative DFT approach is employed to study elastic properties of the FeCrNi medium-range entropy alloys. It is based on our recent and systematic work on the phase stability of both FCC and body-centered-cubic (BCC) Fe-Cr-Ni magnetic alloys using a combination of first-principles constructed Cluster Expansion (CE) Hamiltonian with exchange Monte-Carlo simulations at a finite temperature [41].

The new approach allows us to investigate not only the free energy but also the disorder-order transition of alloys as a function of composition and temperature in terms of Warren-Colley [42,43] short-range order (SRO) effects between different pairs of atoms. The theoretical expression of SRO parameters has recently been derived for MCAs in a matrix formulation [44–47]. The chemical SRO parameter $\alpha_n^{A,B}$ between two species A and B for the n -th nearest neighbor shell can be defined as follows:

$$\alpha_n^{A,B} = 1 - \frac{y_n^{A,B}}{x_A x_B} \quad (2)$$

where $y_n^{A,B}$ denotes the pair probability and x_A, x_B are the concentration of A and B atoms, respectively. Segregation between A and B components gives rise to positive $\alpha_n^{A,B}$ whereas the negative value of $\alpha_n^{A,B}$ means that there is a chemical ordering between them. When $\alpha_n^{A,B} = 0$, A and B atoms are found to be randomly distributed in alloys. Fig. 1a and 1b show the atomistic configurations of medium-range and equiatomic FeCrNi alloys obtained from the present Monte-Carlo simulations of the 9×9×9 FCC supercell for two temperatures: 300 K (Fig. 1a) and 2000 K (Fig. 1b), respectively.

For the practical study of elastic constants in the FeCrNi system from first-principles methods, it is more convenient to reduce the supercell size 9×9×9 to 3×3×3 (Fig. 1c and 1d) in order to balance between computational time and accuracy of DFT calculations. Furthermore, for the high-temperature disordered configurations, the symmetry of the supercell is very low (space group $P1$) due to the random distribution of atoms in the supercell. Here, for obtaining the individual components of the elastic constants matrix, we applied the method based on the deformation of an unstrained structure and the analysis of the changes in the total energy, E_{tot} , computed using DFT as a function of strain [48–51]. The deformation leads to a change in the total energy of the crystal according to the following expressions:

$$U = \frac{E_{tot} - E_0}{V_0} = \frac{1}{2} \sum_{i=1}^6 \sum_{j=1}^6 C_{ij} \varepsilon_i \varepsilon_j \quad (3)$$

where E_0 is the total energy of the unstrained lattice, V_0 is the volume of the undistorted cell and the C_{ij} are the elements of the elastic constant matrix with a notation that follows standard convention. Both i and j run from 1...6 in the sequence $\{xx, yy, zz, yz, xz, xy\}$. For each considered deformation, 8 magnitudes of strain ($\pm 0.2\%$, $\pm 0.4\%$, $\pm 0.6\%$, $\pm 0.8\%$) were applied. The dependencies of the total energy on the deformation were then fitted to quadratic equations and the respective elastic constants were obtained.

To study the elastic properties of Fe-Cr-Ni alloys at high-temperature configuration (T=2000 K), strains were applied for 9 different deformation modes:

$$\begin{aligned} \varepsilon_1 &= \{xx, 0, 0, 0, 0, 0\} \\ \varepsilon_2 &= \{0, yy, 0, 0, 0, 0\} \\ \varepsilon_3 &= \{0, 0, zz, 0, 0, 0\} \\ \varepsilon_4 &= \{xx, yy, 0, 0, 0, 0\} \\ \varepsilon_5 &= \{xx, 0, zz, 0, 0, 0\} \\ \varepsilon_6 &= \{0, yy, zz, 0, 0, 0\} \\ \varepsilon_7 &= \{0, 0, 0, yz, 0, 0\} \\ \varepsilon_8 &= \{0, 0, 0, 0, xz, 0\} \\ \varepsilon_9 &= \{0, 0, 0, 0, 0, xy\} \end{aligned}$$

This allowed obtaining 9 elements of the elastic constant matrix:

$$(C_{ij}) = \begin{bmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ C_{12} & C_{22} & C_{23} & 0 & 0 & 0 \\ C_{13} & C_{23} & C_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{66} \end{bmatrix} \quad (4)$$

Note: In this study, we assumed that the elements of the elastic constant matrix other than C_{11} , C_{12} , C_{13} , C_{22} , C_{23} , C_{33} , C_{44} , C_{55} , C_{66} are equal to zero. Based on our previous study with structures with low symmetry [51], the values of those elements are usually much smaller than C_{11} , C_{12} , C_{13} , C_{22} , C_{23} , C_{33} , C_{44} , C_{55} , C_{66} and can therefore be neglected. Therefore, the lack of those constants should not significantly influence the predictions of the overall elastic properties of alloys. For the low-temperature configuration (T=300 K), the elastic tensor matrix elements (4) has been computed by direct diagonalisation following the tetragonal symmetry as it will be discussed in the Modelling section.

Afterward, we applied the calculation method of the anisotropy of Young's modulus and Poisson's ratio proposed by Wrobel et al. [38] to investigate the anisotropy of elastic properties. In order to obtain the theoretical values of elastic moduli for polycrystalline materials, the Reuss-Voigt-Hill method has been employed [52]. The detailed procedure can be found in Section 4 of the Supplementary Materials.

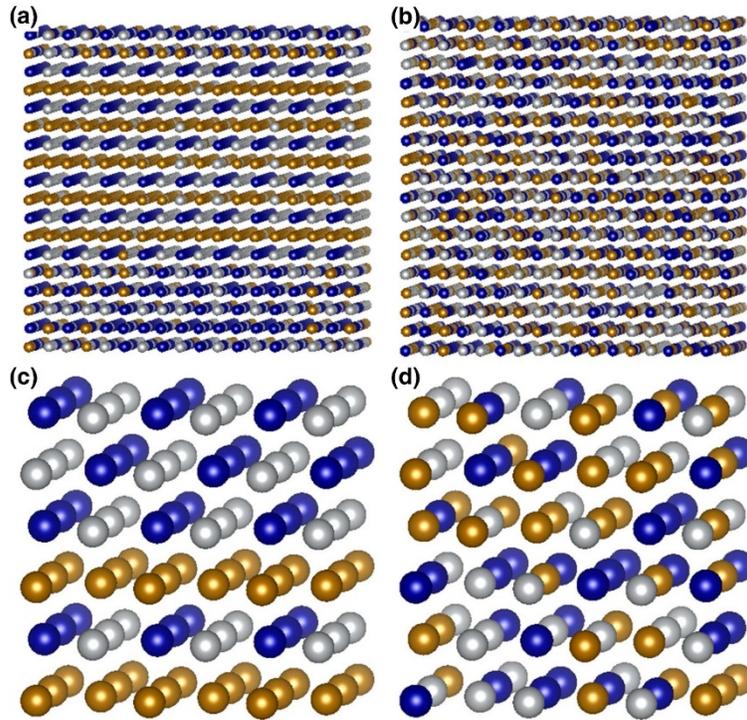


Fig. 1 Monte-Carlo simulations of FCC supercell configurations for equiatomic FeCrNi alloys with different size and temperature using DFT based CE Hamiltonian: (a) $9 \times 9 \times 9$, 300 K; (b) $9 \times 9 \times 9$, 2000 K; (c) $3 \times 3 \times 3$, 300 K; (d) $3 \times 3 \times 3$, 2000 K. The color code for Fe atoms is orange, Cr: blue and Ni: grey

2.4 Microstructure characterization

The microstructure characterizations were performed on the samples sectioned from the fractured tensile bars using electrical discharge machining. The samples were metallographically polished before electron backscatter diffraction (EBSD) test on an HKL EBSD detector based on a scanning electron microscope (SEM, TESCAN MIRA 3, Czech Republic). The SEM parameters for the EBSD were set to a voltage of 20 kV, a current of 25 nA, and a step size of 1.5 μm . The EBSD data analysis was carried out with HKL Channel 5 software. To avoid ambiguous grain boundaries, misorientation angles less than 2° were ignored during the analysis. The thin foils for scanning transmission electron microscope (STEM) observation were mechanically polished to a thickness of $\sim 80 \mu\text{m}$ before the twin-jet electropolishing using a constant of 150 mA in a solution of 5% perchloric acid and 95% methanol cooled to -30°C . The bright-field TEM observation was undertaken on a Tecnai G² F30 microscope operated at 300 kV. The atomic-resolution high-angle annular dark-field STEM (HAADF-STEM) images were performed on an aberration-corrected Titan 60-300 microscope at a voltage of 300 kV. The collection half-angle of the HAADF detector ranging from 60 to 290 mrad was used, with the convergence half-angle of 21.4 mrad, giving a probe size of $\sim 1.2 \text{ \AA}$. The dilatation field of the lattice was analyzed with the geometric phase analysis (GPA) method on the software Strain++ [53], during which a dislocation-free region was chosen as a reference.

Needle-shaped samples for atomic probe tomography (APT) were prepared by lift-out and annular milled in an FEI Scios focused ion beam (FIB)/SEM. The APT characterizations were performed in a local electrode atom probe (CAMEACA LEAP 5000 XR). The specimens were analyzed at 70 K in voltage mode, at a pulse repetition rate of 200 kHz, a pulse fraction of 20%, and an

evaporation detection rate of 0.3% atom per pulse. The 3D reconstructions and data analysis were performed on Imago Visualization and Analysis Software (IVAS) version 3.8.

3. Experimental results

In this section, we first presented the microstructure and mechanical performance of the alloy at 293 K and 15 K. We then presented the analysis of the *in situ* neutron diffraction spectra including the lattice strain, single-crystal elastic constants, the evolution of stacking fault probability (SFP) and dislocation density. Post-mortem TEM characterization was presented afterward.

3.1 Initial microstructure

Fig. 2 shows the micro to nanoscale microstructure of the virgin FeNiCr alloy characterized by SEM-based BSE, EDS, EBSD, HRTEM, and APT. According to the EBSD inverse pole figure (IPF) map on the plane perpendicular to the loading direction (Fig. 2a), the alloy is composed of large equiaxed grains with annealing twins. The average grain size of $\sim 23.4 \mu\text{m}$ was determined by performing the line-intercept method on the EBSD maps excluding the annealing twin boundaries. In Fig. 2b, the band contrast map was overlapped with the boundaries map of Fig. 2a. The low-angle grain boundaries (LAGBs) were defined as misorientations with $15^\circ \geq \theta \geq 2^\circ$ (shown in red lines) while the high-angle grain boundaries (HAGBs) comprise misorientations larger than 15° (shown in black lines). The annealing twin boundaries (TBs) are defined as $\Sigma 3=60^\circ \{111\}$ (shown in blue lines). The fraction of LAGBs is very low (less than 2%) and most of the boundaries were HAGBs. In addition to grain boundaries, a large fraction of annealing TBs was observed. SEM-BSE and corresponding EDS analysis results (Fig. 2c) show a small amount of Cr-rich phase located at grain boundaries. Typical bright-field TEM images of the annealing twin structure are shown in Fig. 2d. Two straight and parallel twin boundaries can be identified with a spacing distance of $\sim 2.18 \mu\text{m}$. The twin relationship is confirmed by the corresponding selected area diffraction (SAED) pattern inserted in Fig. 2d.

The chemical homogeneity of the alloy matrix was confirmed by APT analysis at the atomic scale. Fig. 2e displays the three-dimensional (3D) elemental maps of the three constituent elements, Fe, Cr, and Ni, from a reconstructed volume of $50 \times 50 \times 140 \text{ nm}^3$ containing ~ 12 million ions. There is no apparent elemental segregation in the tested volume. The tested region was found to have a calculated composition of Fe 34.7, Ni 31.8, and Cr 33.5 (at.%), showing an acceptable match to the bulk composition obtained from the ICP-MS. Furthermore, the homogeneity of the atomic distribution of the alloy was also evaluated with the chi-squared statistics with a frequency distribution analysis (FDA) shown in Fig. 2f. The curves from the binomial simulation match well with the curves obtained from the experiments, indicating a randomly distributed solid solution. The parameters used for qualifying the fit are shown in the insert table in Fig. 2f, the normalized homogenization parameter, μ , for all three constituent elements are very close to 0, confirming their random distribution [54].

Besides, to determine if short range orders (SROs) exist in the present alloy, we took over 20 HR-STEM images along different zone axis on the undeformed sample. Two of them are shown in Fig. 2g and 2h, the inset images are the corresponding two-dimensional fast Fourier transforms (FFT) of the HRTEM images. As reported in Refs. [55–57], the existence of SROs can be confirmed by the streaking in the FFT images. However, no such features were captured in our FFT images. From this analysis as well as the APT data, it appears that SROs do not exist in the present alloy.

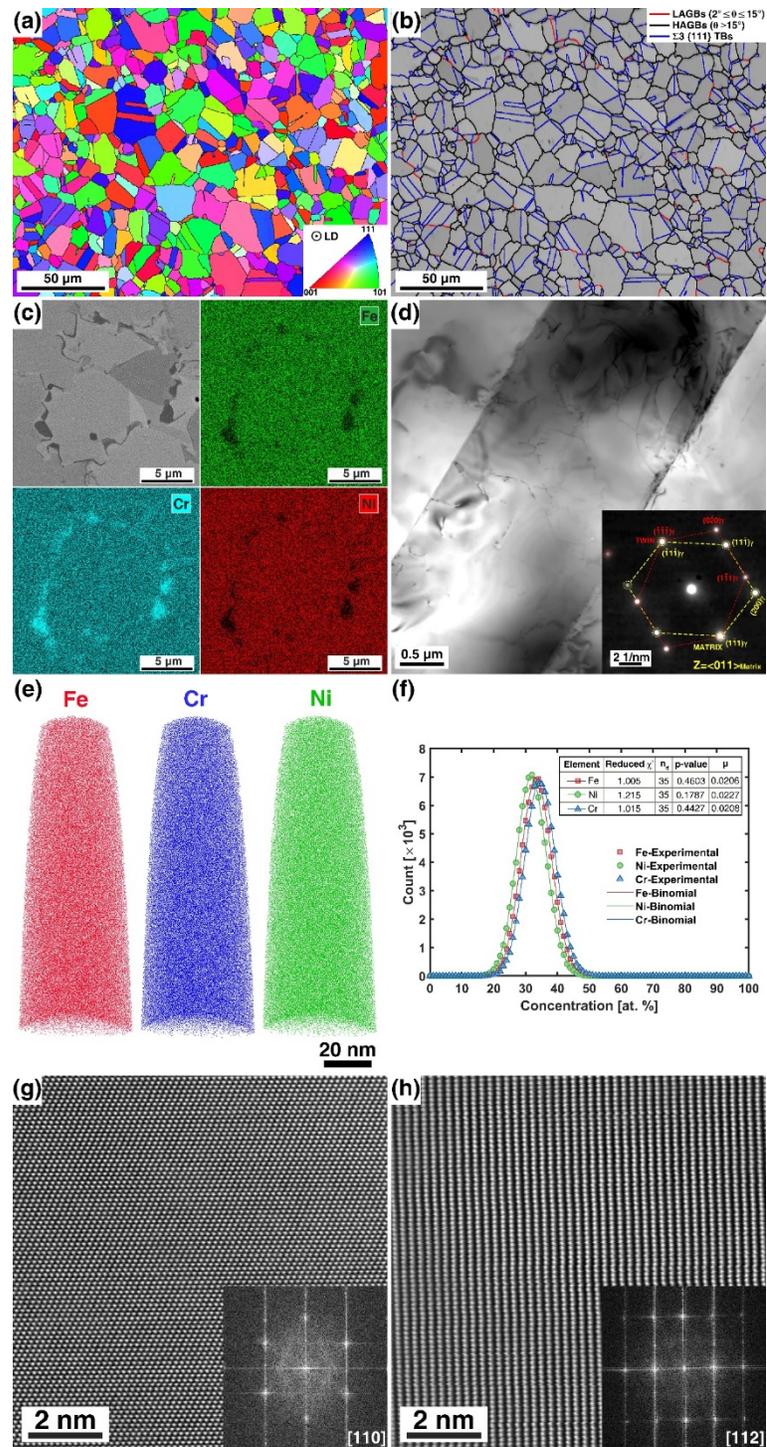


Fig. 2 Microstructure characterization of the virgin sample: (a) EBSD map (inverse pole figure) perpendicular to extrusion direction (ED); (b) Band contrast map overlapped with boundaries map of (a), the red, black, and green lines in the boundary map represents the low-angle grain boundaries (LAGBs), high-angle grain boundaries (HAGBs), and annealing twin boundaries (TBs, $\Sigma 3 \{111\}$); (c) SEM-BSE images and corresponding elemental mapping of Fe, Cr, and Ni obtained from EDX analysis; (d) typical bright TEM image and SAED pattern take along [110] zone axes; (e) Three-dimension APT tip reconstructions of Fe, Cr, and Ni atom; (f) Frequency distribution analysis of the three constituent elements and corresponding parameters used for qualifying the fit; (g) and (h) HRSTEM images and the corresponding FFT images of the alloy taken from [110] and [112] zone axis, respectively.

3.2 Tensile properties

Fig. 3a shows the engineering and true stress-strain curves of the FeCrNi alloy at 293 K and 15 K. The alloy shows a high YS of 651 ± 12 MPa and UTS of 1020 ± 3 MPa, as well as a great elongation of 0.48 ± 0.05 at 293 K. The mechanical properties of the alloy, were then compared with other high strength steels [58] and single or multiphase MEAs/HEAs as shown in Fig. 3b, in which the YS was plotted with respect to total elongation [4–7,11,59–65]. The FeCrNi alloy shows an advantage in achieving high YS and large elongation combination compared to other MCAs at 293 K.

At 15 K, the YS of the FeCrNi alloy increased to 1092 ± 27 MPa, the UTS increased to 1451 ± 2 MPa, while the total elongation decreased to 0.18 ± 0.01 . Corresponding values of the strength and ductility are listed in Table 1. We have also listed the mechanical properties of several HEA/MEA or FCC alloys at 15 K in Table 1. The YS of FeCrNi alloy is highest among the listed alloys, although its elongation is lower.

Table 1. Uniaxial tensile properties of the FeCrNi alloy deformed at 293 K and 15 K

Alloy	Temperature (K)	YS (MPa)	UTS (MPa)	Elongation
FeCrNi	293	651 ± 12	1020 ± 3	0.48 ± 0.05
FeCrNi	15	1092 ± 22	1451 ± 2	0.18 ± 0.01
FeCoCrNiMo _{0.2} [14]	15	710	1423	0.42
CrMnFeCoNi [66]	15	740	2500	0.62
316LN stainless steel [67]	4.2	1045	1528	0.33

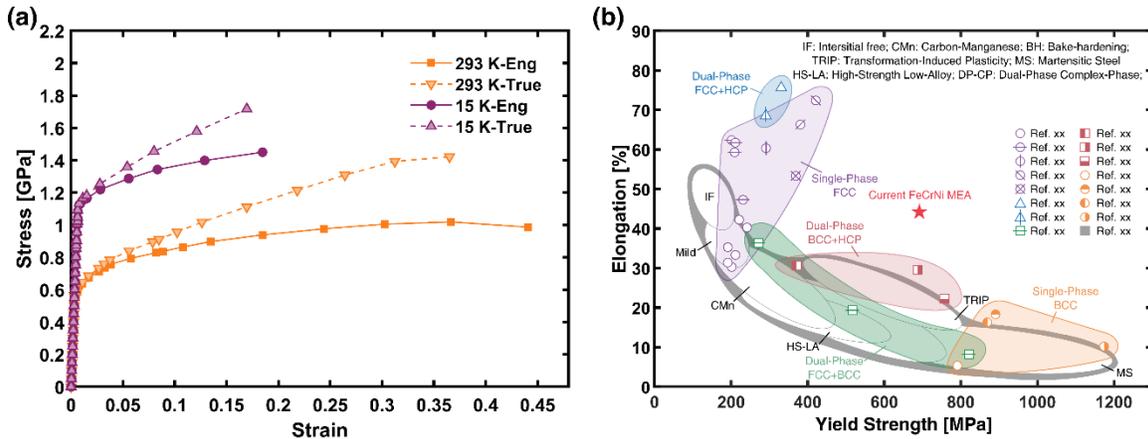


Fig. 3 (a) Engineering and true stress-strain curves of the alloy deformed at 293 K and 15 K; (b) Yield strength-elongation comparison among current FeCrNi MEA, several high-strength steels and single or multi-phase MEAs/HEAs.

3.2 Neutron diffraction spectra

The *in situ* neutron diffraction patterns during tensile testing at 293 K and 15 K plotted with respect to true stress were shown in Fig. 4a and 4b, respectively. Five reflections of $\{111\}$, $\{200\}$, $\{220\}$, $\{311\}$, and $\{222\}$ from the single FCC phase can be observed at both 293 K and 15 K before deformation. During and after the tensile testing at both temperatures, no new peaks appeared, indicating the FCC structure was stable and maintained as a single FCC phase solid solution under loading. The lattice parameter (a_0) was obtained by performing Rietveld refinement on neutron diffraction patterns. The lattice parameter decreased slightly from 3.602 \AA to 3.594 \AA as the temperature decreased from 293 K to 15 K due to the shrinkage of atomic bands [68].

The measured lattice strain from five crystallographic planes of ($\{111\}$, $\{200\}$, $\{220\}$, $\{311\}$, and $\{222\}$) along axial and radial direction were plotted as a function of true stress in Fig. 5a (293 K) and 5b (15 K). The uncertainties in the measured internal strains were approximately 30 microstrain [69]. The measured bulk elastic Young's modulus (E_M) at different temperatures were obtained by linear fitting the true stress and strain curves at the elastic stage. Similarly, the elastic constants of each orientation (E_{111} , E_{200} , E_{220} , and E_{311}) were then obtained by linear fitting the lattice strain and true stress before yielding (Table 2). After yielding, the orientation-dependent yielding behaviors were observed at both temperatures. As indicated in Fig. 5a and 5b, the $\{111\}$ grain family has the highest stiffness (E_{111} of 248.1 GPa at 293 K and 260.4 GPa at 15 K). It, however, showed the earliest yielding behavior (~ 550 MPa at 293 K and ~ 1000 MPa at 15 K). Meanwhile, among all 4 grain families, $\{200\}$ showed the lowest stiffness (E_{200} of 148.6 GPa at 293 K and 162.3 GPa at 15 K) and a delayed yielding behavior (~ 730 MPa at 293 K and ~ 1150 MPa at 15 K). The varied stiffness and yielding behaviors among different grain planes can be ascribed to the elastic and plastic anisotropy of the crystals. After yielding of some stiff grain families (e.g. $\{111\}$), the external stress gradually transferred to other soft grain families (e.g. $\{200\}$).

Table 2 Experimentally measured elastic properties of the FeCrNi alloy at different temperatures

Temp. [K]	E [GPa]	E_{111} [GPa]	E_{200} [GPa]	E_{220} [GPa]	E_{311} [GPa]	ν_{111}	ν_{200}	ν_{220}	ν_{311}	ν	G [GPa]
293	200.5	248.1	148.6	220.7	185.9	0.256	0.339	0.314	0.335	0.292	77.6
15	237.2	260.4	162.3	225.7	197.2	0.233	0.320	0.282	0.302	0.281	92.6

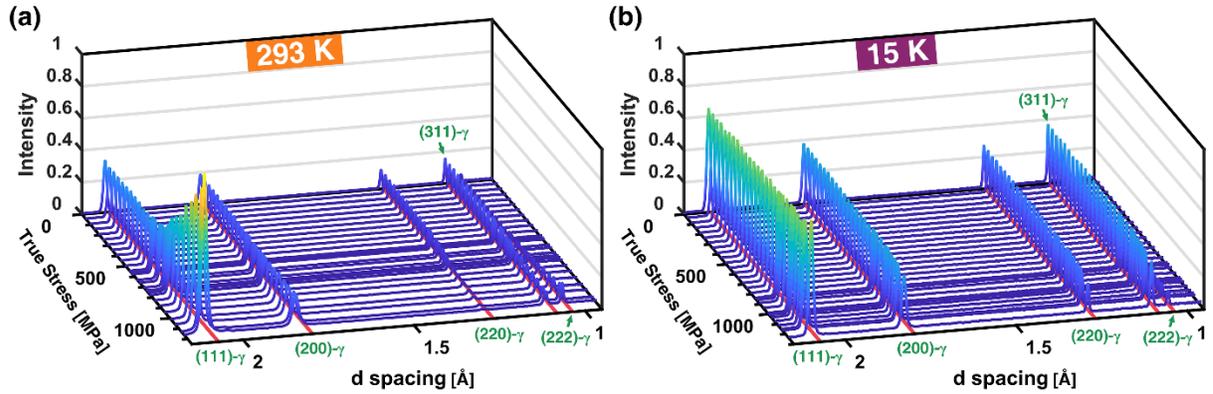


Fig. 4 *In situ* neutron diffraction spectra collected during deforming at (a) 293 K and (b) 15 K.

3.3 Single-crystal elastic constants calculation

During elastic deformation, the lattice parameter obtained at axial and radial directions increased linearly with true stress. Their slopes at radial and axial directions were obtained by linear fitting and the ratio of the two slopes determines the Poisson's ratio (ν). Then the shear modulus (G) was obtained via $G = E/2(1 + \nu)$. The drop of deformation temperature increased the stiffness of the alloy as the E_{hkl} at all four orientations increased to varying degrees.

To better understand the underlying elastic deformation behavior of the alloy at different temperatures, several materials properties, including macroscopic elastic, shear, and bulk moduli

(E_M , G_M , and K_M), were calculated from diffraction elastic moduli (E_{hkl}) and Poisson's ratio (ν_{hkl}) using Voigt [70], Reuss [71], and Kroner [72] model. The detailed procedure can be found in Section 1 of the Supplementary Materials. In Fig. 6a and 6b, the two reciprocal diffraction elastic constants ($1/E_{hkl}$ and ν_{hkl}/E_{hkl}) obtained from experimental elastic lattice strain and calculated with Voigt, Reuss, and Kroner model are plotted with respect to the elastic anisotropy factor ($A_{hkl} = \frac{h^2k^2 + h^2l^2 + k^2l^2}{(h^2 + k^2 + l^2)^2}$) at 293 K and 15 K, respectively. The fitting results indicate that among

all three models, the Kroner model shows the best agreement with the experimental results at both 293 K and 15 K. The Voigt model simply assumes that all grains were uniformly strained, but the force among grains cannot meet the equilibrium. While in the Reuss model, homogeneous stress was assumed to be applied to all grains, but the distorted grains cannot fit together. Therefore, due to their simplicity, the Voigt and Reuss model are generally used to define the upper and lower bounds of the diffraction and isotropic macroscopic elastic constants. By contrast, the Kroner model provides a more accurate estimation of elastic properties after considering the orientation dependence of elastic parameters. The single-crystal elastic constants, elastic, polycrystalline moduli, and Poisson's ratio at 293 K and 15 K calculated by this method are listed in Table 4. The values of C_{11} and C_{44} decreased slightly as the temperature decreased from 293 K to 15 K, while C_{12} remains nearly constant.

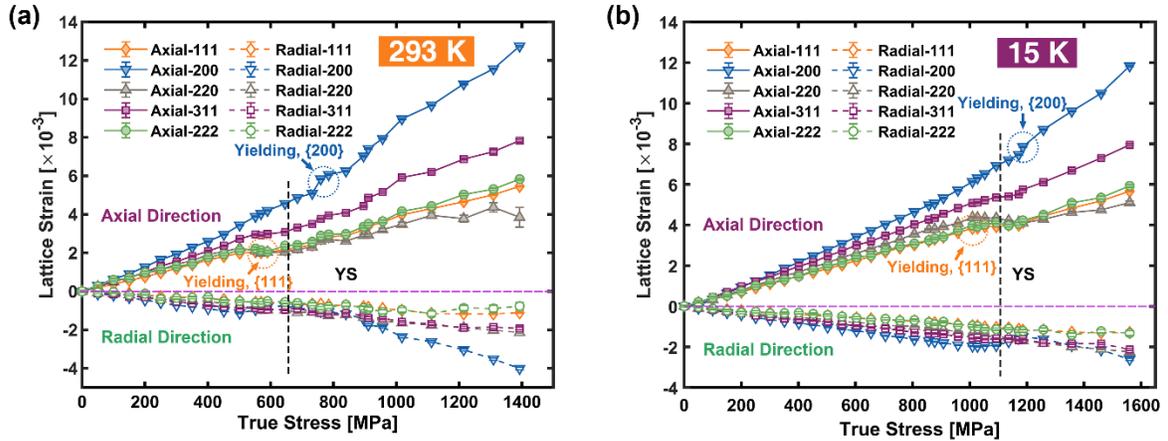


Fig. 5 Lattice strain evolution of crystallographic planes of {111}, {200}, {220}, {311}, and {222} from axial and radial directions during deforming at (a) 293 K and (b) 15 K.

The orientation-dependent elastic properties of the FeNiCr alloy at 293 K (determined from neutron diffraction and DFT simulation results) were illustrated in Fig. 7. To calculate the elastic properties in any direction, the fourth-order elastic tensor was transformed in a new basis with Eq. (S20). The experimentally determined elastic properties of the alloy were illustrated with the three-dimensional (3D) surfaces (left column). The experimental results along directions at XY, XZ, and YZ planes were shown in the middle column by 2D contours. The Young's modulus is shown in Fig. 7a and 7e. The maximum and minimum values of 302 GPa and 119 GPa were observed at $\langle 111 \rangle$ and $\langle 100 \rangle$ direction, respectively. The ratio of maximum-to-minimum elastic modulus of 2.5 indicates the high anisotropy property of the alloy. The 3D surfaces of shear modulus and Poisson's ratio were shown in Fig. 7b and 7f, respectively. The translucent outer surface represents the maximum value while the solid surface inside shows the minimum values. The maximum and minimum values were shown with dashed and solid lines in the corresponding 2D contours. The maximum value of the shear modulus (127 GPa) appeared at $\langle 100 \rangle$ direction whereas the minimum value of 55.3 GPa is in $\langle 110 \rangle$ direction, yielding the ratio of the maximum to the minimum shear modulus of 2.3 (Fig. 7c and 7g). For Poisson's ratio, the maximum value of 0.4 ($\langle 100 \rangle$ direction)

while the minimum value is approaching 0 (Fig. 7e and 7f). In Fig. 7g and 7h, the linear compressibility (LC) has a value of 1.9 TPa^{-1} , showing negligible anisotropy in all directions.

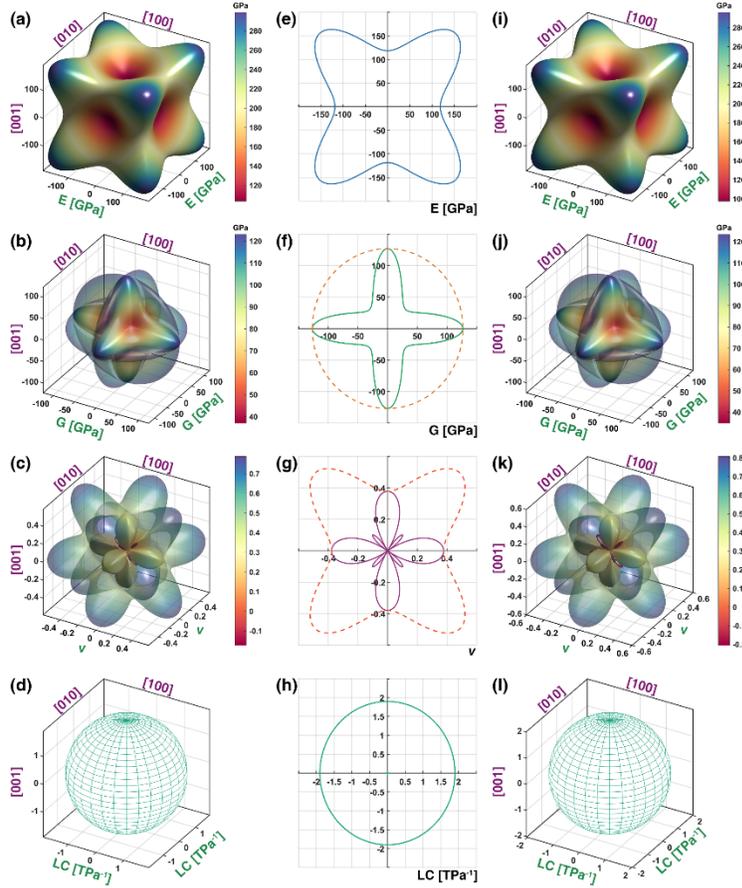


Fig. 7 Elastic properties of the FeNiCr alloy at 293 K determined via *in situ* neutron diffraction measurement (a-h) and DFT calculation (i-l). The magnitude with respect to the directions in three dimensions for: (a)(i) Young's modulus, (c)(j) shear modulus, (e)(k) Poisson's ratio, and (g)(l) linear compressibility, respectively. The maximum and minimum values of shear modulus and Poisson's ratio are represented by two surfaces. The magnitude with respect to directions of XY, XZ, and YZ plane for (b) Young's modulus, (d) shear modulus, (f) linear compressibility, and (h) Poisson's ratio, respectively. The maximum and minimum values of shear modulus and Poisson's ratio are represented by dashed and solid lines, respectively.

3.5 Stacking fault probability

The SFP measures the amount of stacking faults formed during deformation and allows the determination of the stacking fault energy (SFE) [8,14] of the alloy. The detailed calculation procedure of SFP and SFE can be found in Section 2 of the Supplementary Materials. The measured SFP evolution of the FeNiCr alloy at 293 K and 15 K is compared with another high entropy alloy (FeCoCrNiMo_{0.2}) (Fig. 8a) [73]. At high strain levels, the FeCoCrNiMo_{0.2} showed a very high level of SFP. Its maximum value reached 2.9×10^{-2} at 77 K and even increased to 5.1×10^{-2} at 15 K. The alloy shows a very low level of SFE of 17 mJm^{-2} and 11 mJm^{-2} at 77 K and 15 K, respectively. By contrast, the SFP of FeNiCr alloy is very low (below 7×10^{-3}) at both temperatures. According to Eq. (S13), the SFE of the alloy was estimated to be $63 \pm 4 \text{ mJm}^{-2}$ at 293 K and $47 \pm 3 \text{ mJm}^{-2}$ at 15 K.

Generally, the SFE of an alloy serves as one of the most crucial parameters determining the dominant deformation mechanisms. The strain hardening effects were mainly controlled by dislocation motion when the SFE exceeds 45 mJm^{-2} . As the SFE decreased to the range of $18 \sim 45$

mJm^{-2} , twinning is preferably to occur. While phase transformation, from the parent FCC to new-born phases with hexagonal close-packed (HCP) and/or body-centered tetragonal (BCT) structured may occur if the SFE is further decreased to be lower than 18 mJm^{-2} [28,74]. This relationship is well-supported in previous studies [14,28]. The thermodynamic calculation results indicate that the SFE of the FeNiCr alloy is in the range of $50\sim 60 \text{ mJm}^{-2}$ [75]. This is also confirmed in Refs. [76,77], where the high SFE of the FeNiCr was predicted to be $>50 \text{ mJm}^{-2}$ by large-scale atomic simulations. These previous studies agree with our calculation based on the diffraction data analysis. The high SFE of the FeNiCr alloy ($63\pm 4 \text{ mJm}^{-2}$ at 293 K and $47\pm 3 \text{ mJm}^{-2}$ at 15 K) suggests that its deformation behavior is mainly controlled by the dislocation motion, while the stacking fault, twins, and phase transformation are less likely to occur during deformation.

The high SFE of the FeNiCr alloy can be attributed to two reasons: (1) the low configurational entropy and (2) the high concentration of Cr and Ni element. Zaddach et al. [77] applied diffraction methods and first principles to investigate the SFE of a series of MCAs (FeCoNiCrMn) and the results indicated that the SFE decreases with the increase of element complexity, i.e., constituent number or configurational entropy. On the other hand, Refs. [78,79] indicate that the SFE of an alloy is the combined effect of each constituent element. The same element can influence the SFE differently in different alloy systems. For the FeCoNiCrMn alloy system, the SFE can be increased by increasing Ni contents as the high intrinsic SFE of Ni ($\sim 125 \text{ mJm}^{-2}$) [80]. This also agrees with the study of Bonny et al. [76], which suggests that the SFE of FeNiCr alloy can be significantly increased by increasing Cr and Ni content.

3.6 Dislocation density evolution

The dislocation density evolution of the alloy during deformation was calculated with the modified Williamson-Hall method [81]. The detailed procedure for dislocation density calculation can be seen in Section 3 of the Supplementary Materials. The calculated dislocation density at both temperatures is shown in Fig. 8b. The evolution of dislocation density showed a very similar pattern at both temperatures. Both curves fluctuate slightly at around $6 \times 10^{13} \text{ m}^{-2}$ before yielding, after which both curves increase almost linearly upon further straining. At 293 K, the dislocation density of $1.74 \times 10^{15} \text{ m}^{-2}$ was achieved at true stress of 1392 MPa and true strain of 0.31. At 15 K the dislocation density reached $7.93 \times 10^{14} \text{ m}^{-2}$ at true stress of 1576 MPa and true strain of 0.12.

Meanwhile, the dislocation evolution is closely related to the texture development during tensile loading. The intensity of each reflection ($\langle 111 \rangle$, $\langle 200 \rangle$, $\langle 220 \rangle$, $\langle 311 \rangle$, and $\langle 222 \rangle$) was normalized with that of the stress-free state and their evolution with true stress at 293 K and 15 K are shown in Fig. 8c and 8d, respectively. At both temperatures, the peak intensity curves changed very little during the elastic stage while they started to vary after the yielding points. This originates from the difference in grain rotation in response to external loading. At 293 K, after yielding, (111)//LD and (222)//LD orientated grains gradually rotated towards the loading direction, making their peak intensity increase almost linearly with the increase of true stress during subsequent straining. By contrast, the intensity of (200) peak maintained at a similar level of ~ 0.8 after a slight dropping. The intensity of the other two peaks, (311) and (220), decreased to 0.43 and 0.09 as grains with these orientations gradually rotated away from LD. A similar phenomenon was also observed in 15 K (Fig. 8b) and reported in Refs. [6,8]. In the present study, the (111)//LD texture was used as a measure of the dislocation activity as the texture development is characteristic of dislocation slip during plastic deformation [66]. The highest (111) intensity reached 2.62 at 293 K, comparing with a much lower value of 1.29 at 15 K. Meanwhile, at 293 K the texture developed at a faster pace (with a slope of $\sim 2.35 \times 10^{-3} \text{ MPa}^{-1}$) than that at 15 K (with a slope of $\sim 0.67 \times 10^{-3} \text{ MPa}^{-1}$). The slow texture change at 15 K also explains the lower strength enhancement after yielding and deterioration of the ductility observed at 15 K (Fig. 3). The inactive grain rotation and

slow texture evolution limited the dislocation motions to well-orientated grains and led to the inability of catering to larger external strain [82,83]. Meanwhile, fewer slip systems can be activated in those “not-so-good-oriented” grains, leading to a much lower dislocation density achieved at 15 K. This result is in good agreement with the mechanical performance (Fig. 3a) and the dislocation density evolution (Fig. 8b).

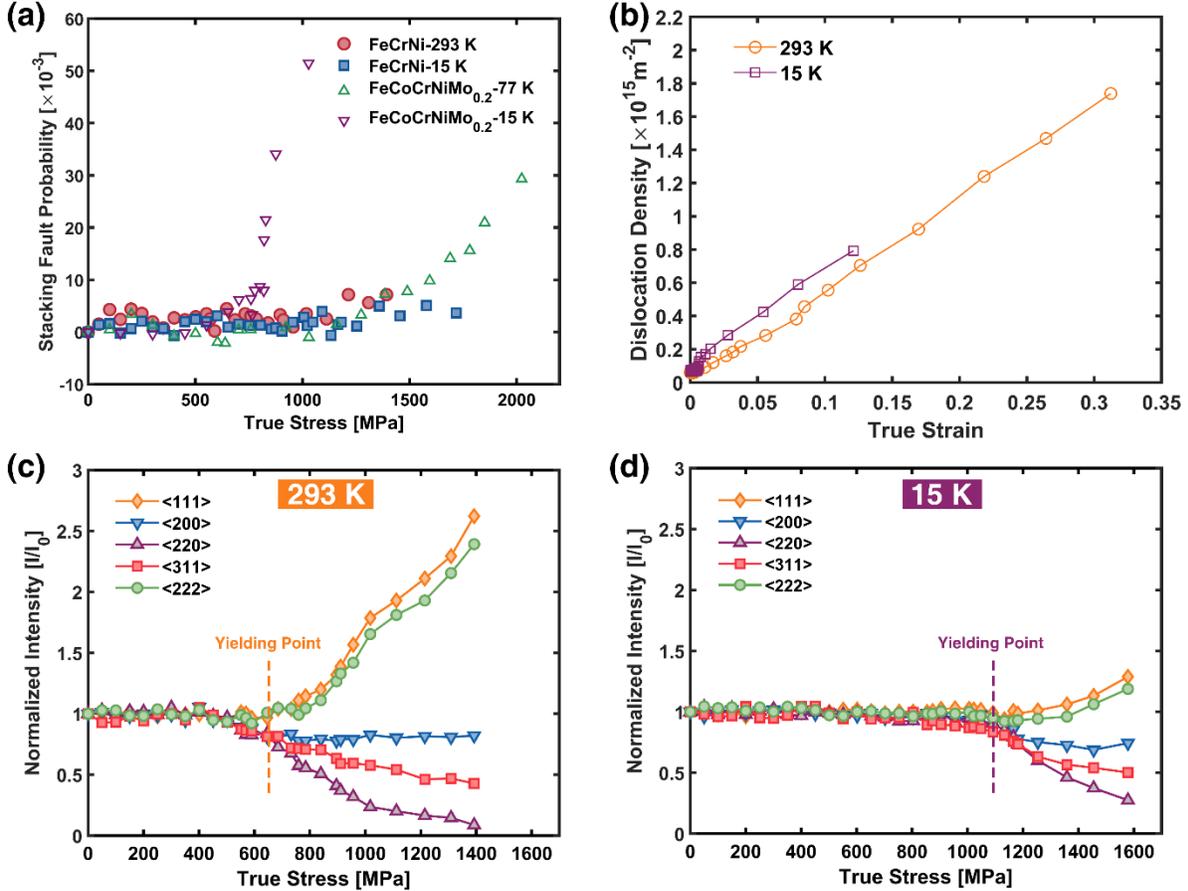


Fig. 8 Microstructure evolution during straining at 293 K and 15 K: (a) Comparison of stacking fault probability (SFP) evolution between the FeNiCr alloy and FeCoCrNiMo_{0.2} alloy at different temperatures; (b) Dislocation density evolution; The normalized peak intensity evolution of {111}, {200}, {220}, {311}, and {222} during deforming at (c) 293 K and (d) 15 K.

3.6 TEM characterization of the strained samples

To further reveal the underlying deformation mechanisms, post-mortem TEM characterizations were performed on the fractured samples deformed at 293 K and 15 K. Fig. 9a shows the bright-field STEM micrograph of the alloy deformed to a low strain level of ~ 0.1 at 293 K, massive parallel shear bands traveling through the whole grain interior were observed. The image on the inset of Fig. 9a is the SAED pattern taken from the area highlighted by the yellow circle, showing the matrix still maintained a stable FCC structure. The shear bands mainly consist of closely arrayed dislocation walls whereas no twins were detected, indicating the alloy deforms by typical planar dislocation glide on {111} planes. The shear bands were magnified in Fig. 9b, showing that the dislocation walls consisted of massive dense parallel primary {111} slip traces. Fig. 9c is the bright-field TEM image taken from the sample sectioned near the fracture surface. Dense dislocation networks were produced between slip traces. Secondary {111} slip occurred and intersected with

the primary slip traces, separating the matrix into small parallelogram blocks. The mean free path of mobile dislocations can be effectively reduced by the concentrated slip bands.

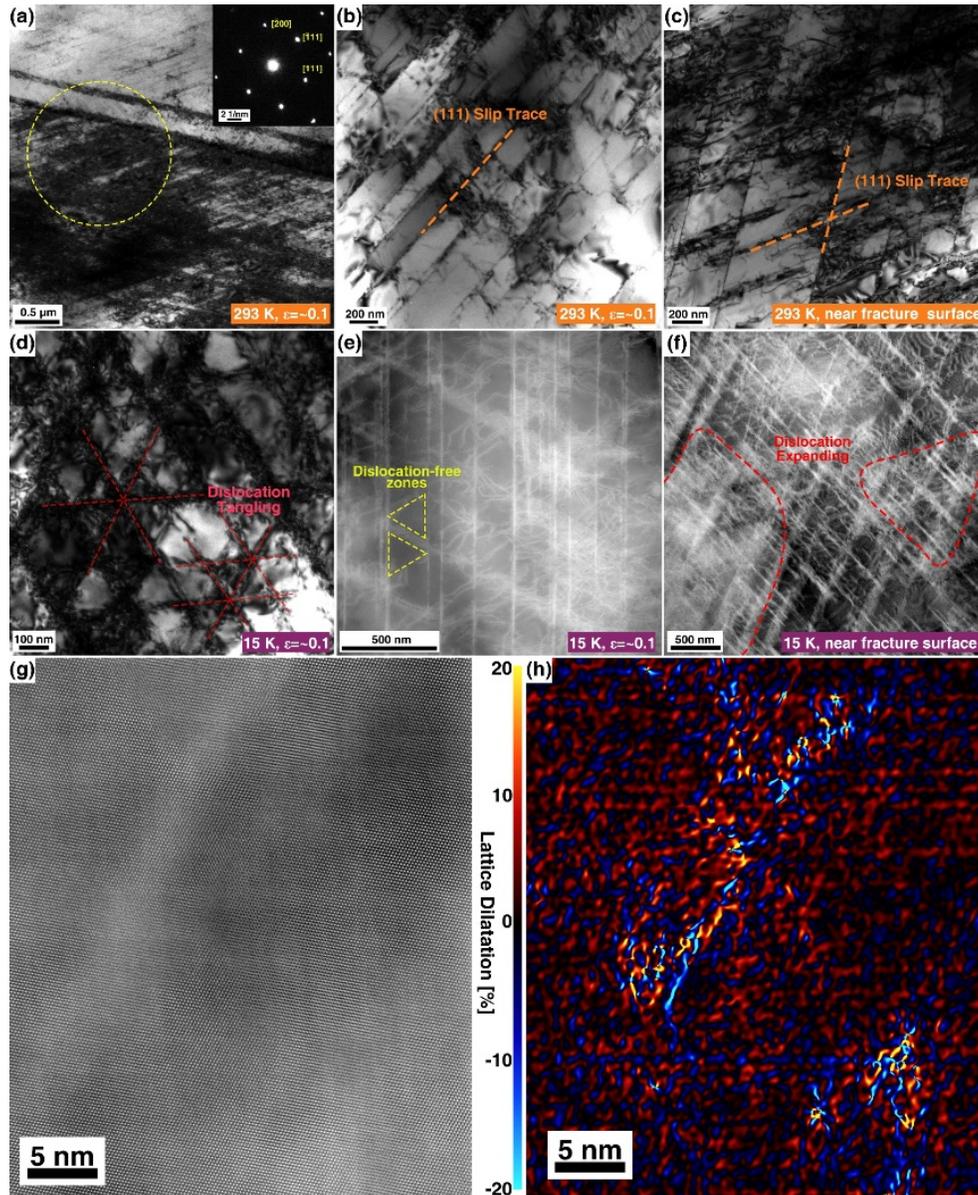


Fig. 9 Deformed microstructure of the alloy at different strain levels and different temperatures, 293 K and 15 K: (a) typical bright TEM image (at strain of ~ 0.1 , 293 K) and corresponding SAED pattern of the area marked by the yellow dashed circle; (b)(c) bright field TEM images at strain of ~ 0.1 and near the fracture surface at 293 K, respectively; (d) bright field TEM image at strain of ~ 0.1 , 15 K; (e)(f) HAADF-STEM images of the deformed structure at strain of ~ 0.1 and near the fracture surface at 15 K, respectively; (g) HRTEM image of the dislocation tangling zone in (e); (h) The geometric phase analysis (GPA) conducted on (g).

Similar dislocation motions were also observed at 15 K. Fig. 9d is the bright-field TEM image showing the microstructure of the alloy deformed to a strain of ~ 0.1 at 15 K. Comparing with Fig. 9b, the secondary slip system is more easily activated at 15 K, more dislocation tangling kinks were observed. Dislocations were preferably gathered around the crossing slip systems and form parallelogram blocks. The interior of the nanosized dislocation substructure shows a relatively lower dislocation density than the block boundaries. The morphology of dislocation networks of

the sample deformed to a strain of ~0.1 and near the fracture surface was further revealed by STEM-HAADF images in Fig. 9e and 9f, respectively. In Fig. 9f, the density of intersecting active slip planes increased significantly as more slip systems were activated, refining the spacing between coplanar slip bands significantly. The concentrated slip bands can hinder dislocation slip on parallel slip bands by increasing the passing stresses. Furthermore, rapid dislocation multiplication occurred in both dislocation walls and the small dislocation-free zones (Fig.9e), thickening the dislocation walls effectively and gradually expanding dislocations to the whole block interior (Fig. 9f). Fig. 9g displays the HAADF image of a slip trace junction in Fig. 9f. Fig. 9h is the lattice dilatation resulting from the presence of a high strain field, obtained from the trace of the lattice distortion matrix via the GPA method [53]. This result identified the crossing slip traces, especially their junctions, mainly consist of tangling dense dislocations accompanied by a high residual strain field. It is also worth noting that at both temperatures, very few short and isolated stacking faults were observed from our STEM observation, which is consistent with our neutron diffraction results in Fig. 8a.

4 Modelling results

4.1 Phase formation parameters

Several thermodynamic parameters related to phase formation including ΔS_{mix} (entropy of mixing), ΔH_{mix} (enthalpy of mixing), T_m (melting point) were calculated (see Section 5 of the Supplementary Materials). Besides, the parameter Ω , which can be applied to predict the solid-solution formation of random MCAs was calculated according to Ref. [84],:

$$\Omega = \frac{T_m \Delta S_{mix}}{|\Delta H_{mix}|} \quad (5)$$

When $\Omega > 1$, the MCAs are mainly composed of solid solutions while $\Omega \leq 1$, the formation of intermetallic compounds or segregations are favored.

Another important parameter in predicting the solid-solution formation is the parameter δ [84], which describes the atomic size difference of the MCAs and can be expressed as follows:

$$\delta = \sqrt{\sum_{i=1}^n c_i \left(1 - \frac{r_i}{\bar{r}}\right)^2} \quad (6)$$

, in which r_i is the atomic radius and $\bar{r} = \sum_{i=1}^n c_i r_i$ is the average atomic radius. According to Refs. [84,85], when $\Omega \geq 1.1$ and $\delta \leq 6.6\%$, stable solid-solution phases can be formed in MCAs.

Furthermore, Guo et al. [86] indicated that the valence electron concentration (VEC) serves as a criterion for determining the lattice structure of the MCAs as it correlated a structure's VEC with its FCC/BCC phase formation. It is defined by:

$$VEC = \sum_{i=1}^n c_i (VEC)_i \quad (7)$$

, where $(VEC)_i$ is the VEC for i th element and can be found at Ref. [86]. When $VEC \geq 8$, FCC structure is more stable while $VEC \leq 6.87$, BCC phases are more stable [87].

Therefore, multiple phase formation parameters can be calculated based on Eqs. (8-10) and the results are shown in Table 3. As can be seen, the FeCrNi alloy has a very high ΔS_{mix} (9.132 J·K⁻¹

$^1\text{mol}^{-1}$), T_m (1906.6 K), and relatively small ΔH_{mix} ($-4.3972 \text{ KJ}\cdot\text{mol}^{-1}$), yielding the high value of Ω (3.9596). Accompanied with a low \mathcal{S} value (only 0.002), the result indicates the alloy can favorably form stable solid-solution phases. Additionally, the VEC of the alloy is calculated to be 7.97, which is very close to the theoretical criterion of forming a single FCC structure [87]. According to the neutron diffraction spectra (Fig. 3) and TEM results (Fig. 2 and 9), a single FCC solid solution phase was observed, in good agreement with the theoretical prediction.

Table 3 Multiple phase formation parameters, \mathcal{S} , ΔH_{mix} , ΔS_{mix} , and Ω of the FeCrNi alloy

Alloy	ΔS_{mix} [$\text{JK}^{-1}\text{mol}^{-1}$]	ΔH_{mix} [KJmol^{-1}]	T_m [K]	Ω	\mathcal{S}	VEC
FeCrNi	9.132	-4.3972	1906.6	3.9596	0.002	7.97

4.2 DFT results

According to the DFT results, up to the melting point, the free energy calculations considering magnetic corrections demonstrate that the FCC phase is stable at the equiatomic composition of FeCrNi alloy, which is in excellent agreement with available experimental data. The atomistic configurations of medium-range and equiatomic FeCrNi alloys obtained from the present Monte-Carlo simulations of the $9\times 9\times 9$ FCC supercell for two temperatures: 300 K and 2000 K are shown in Fig. 1a and 1b, respectively. At 2000 K, the configuration is more related to a disordered distribution of Fe, Cr, and Ni atoms over the simulation cell, whereas at 300 K, the configuration is more related to an ordering configuration. To understand this disorder to order transition, Fig. 10 shows the dependence of the first nearest-neighbor (1NN) SRO parameters of Fe-Cr, Fe-Ni, and C-Ni pairs as a function of temperature. At the high-temperature region, all the values of SRO trend to approach the zero values corresponding to random alloy configurations. For the region of temperature lower than 1000 K, it is found that the SRO parameters for Fe-Cr and Fe-Ni are negative expressing the chemical interactions between these pairs in the ternary FeCrNi alloy. Between them, the SRO parameters for Fe-Cr pairs are more negative than those of Fe-Ni demonstrating a stronger chemical ordering between Fe and Cr. The SRO parameters between Cr and Ni are positive in this temperature range demonstrating that these two atoms did not like each other within 1NN shell of the FCC lattice.

Fig. 1c and 1d show the $3\times 3\times 3$ supercell configurations used for DFT calculations of elastic constants in equiatomic FeCrNi alloys within the present work. They have been generated by using combined first-principles CE Hamiltonian with exchange Monte Carlo simulations at 300 K and 2000 K. Space group symmetry of these configurations are found to be $P1$ and $Pnmm$, respectively. The prediction of orthorhombic symmetry for the 300 K configuration demonstrates that the ordered structure obtained from the present theoretical study is strongly correlated with the SRO effects shown in Fig. 10 at low temperature for the medium-range FeCrNi alloy at equiatomic composition. It is worth noting that the point group symmetry of $Pnmm$ crystal represents a subgroup of the tetragonal structure $P4/mmm$ which has been previously predicted for intermetallic phase Fe_2CrNi from our DFT study in the FCC Fe-Cr-Ni system [41].

The elastic constants calculated by DFT for configurations generated by MC simulations at 300 K and 2000 K MC are shown in Table 4. Note that for the high-temperature (2000 K) configurations with $P1$ symmetry, the elastic constant values were computed by the new method outlined from Eqs. (3) and (4) where the 12 components from 21 independent elastic tensor components are negligible for the random alloy configuration. For the low-temperature configuration (300 K), DFT calculations provide 9 independent elastic constant values according to the orthorhombic group symmetry $Pnmm$. The optimized lattice constants from DFT calculations for the low-temperature configurations are $a=3.5549\text{\AA}$, $b=3.5486\text{\AA}$, and $c=3.6264\text{\AA}$ which are slightly different from the

ones for a cubic cell. The corresponding values for high-temperature configurations are $a=3.5385\text{\AA}$, $b=3.5459\text{\AA}$, and $c=3.5722\text{\AA}$. A larger lattice constant value at low temperature can be explained by magneto-volume effects due to high values of predicted magnetic moments in the ordered FeCrNi alloys. According to our DFT calculations, the average ferromagnetic moments of Fe and Ni sites are $2.1 \mu_B$ and $0.16 \mu_B$, respectively, whereas an average anti-ferromagnetic moment of $\pm 2.2 \mu_B$ was found from Cr sites within the orthorhombic structure $Pnmm$. Note that the magnetic moment value predicted for the Fe site in the Fe_2CrNi structure is also found to be closer to $2.1 \mu_B$ [41]. For the high-temperature configuration, magnetic moments at different atomic sites are found to be randomly distributed and their average values are smaller than those predicted above for the ordered structure as expected. As it can be seen from Table 4, the DFT calculations were performed within different options, either with the lattice and ionic relaxations (denoted as “Relaxed”) or without ionic relaxations (denoted as “Unrelaxed”).

Table 4 Elastic constants and moduli predicted by DFT calculations and compared with experimental data. (More detailed comparison can be found in Table S2, the Supplementary Materials)

FeCrNi		DFT 2000 K	DFT 2000 K	DFT 300 K	DFT 300 K	In situ Exp. 293 K	In situ Exp. 15 K
Symmetry		$P1$	$P1$	$Pnmm$	$Pnmm$		
K-points		$4\times 4\times 4$	$4\times 4\times 4$	$4\times 4\times 4$	$6\times 6\times 6$		
		Relaxed	Unrelaxed	Relaxed	Relaxed		
Elastic Constant [GPa]	C_{11}	210.79	222.45	239.41	237.44	225	220
	C_{12}	141.19	134.8	117.01	116.4	151	134
	C_{13}	136.06	142.6	136.48	137.24	-	-
	C_{22}	200.47	213.16	231.37	229.99	-	-
	C_{23}	127.42	132.09	109.34	108.92	-	-
	C_{33}	206.05	218.31	257.46	259.19	-	-
	C_{44}	123.42	125.36	163.14	163.46	123	127
	C_{55}	122.36	138.84	143.22	142.18	-	-
	C_{66}	122.19	131.67	141.19	140.99	-	-
	C' (average)	35.4	40.7	60.9	60.7	37.0	43.0
Young's Modulus [GPa]	E_{av}	180.83	199.81	248.02	247.12	187.95	201.8
Poisson's Ratio	P_{av}	0.3093	0.2962	0.2429	0.2433	0.3216	0.2932
Polycrystalline Moduli [GPa]	$B_{(VRH)}$	158.33	163.53	161.09	160.77	175.65	162.67
	$G_{(VRH)}$	74.57	82.45	103.62	103.27	76.17	82.35
	$E_{(VRH)}$	192.64	211.12	255.64	254.82	199.06	210.9

From the DFT results, it is found that elastic constants at high temperatures are smaller than the ones under low-temperature configurations, demonstrating the strong effect of disorder with respect to chemical ordering for the latter one. From Table 4, the predicted DFT elastic properties for the disordered configuration generated by MC simulations at 2000 K are in very good agreement with experimental values measured in this work. The elastic properties obtained by DFT are shown in Fig. 7i to 7l, which also closely resembles those measured experimentally. This strongly indicates that the prepared experimental FeCrNi alloy samples are more likely to be the metastable phase

produced by the fabrication technique without annealing treatment, which may prevent the formation of SROs and ordered intermetallic phase predicted by DFT calculations at a low-temperature regime. This also means that the SRO effects shown in Fig. 10 from our modeling work are absent in the present experimental alloys. The absence of the SRO effect is checked by the neutron diffraction results (Fig. 4) and it is found that no other diffuse superlattice peaks can be identified experimentally. Furthermore, this result is well-supported by the APT analysis and the extensive HRTEM analysis (Fig. 2). According to Ref. [57], SRO formation preferably occurred after long-time annealing at high temperatures. In CrCoNi alloy, SROs were observed after annealing at 1000 °C for 120 h [88].

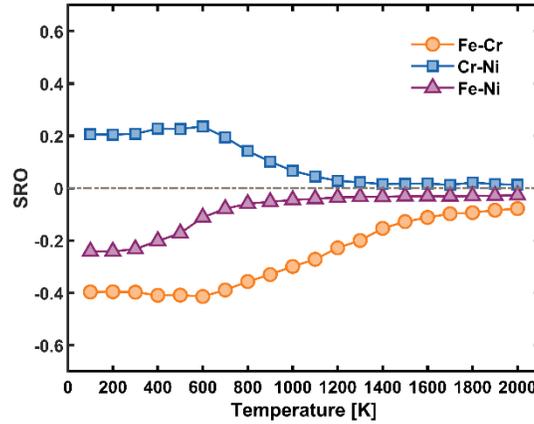


Fig. 10 Dependence of SRO parameters as a function of temperature between the three different pairs in equiatomic FeCrNi alloys.

4.1 Yield strength modeling

For the FeNiCr MEA, the YS can be the accumulative result of several strength contributors including frictional stress (σ_{fr}), initial dislocation density (σ_{dis}), precipitate hardening (σ_{ppt}), and grain boundary strengthening (σ_{gb}) [4]:

$$\sigma_{YS} = \sigma_{fr} + \sigma_{dis} + \sigma_{ppt} + \sigma_{gb} \quad (8)$$

First, the precipitation strengthening can be ignored in the present study. According to the neutron diffraction results shown in Fig. 4, during elastic deformation at both 293 K and 15 K, the alloy keeps a single FCC phase, and no precipitates were detected except a small amount of Cr-rich phases at grain boundaries (Fig. 2c). The bright-field TEM images and corresponding SAED patterns (Fig. 2 and 9) did not observe nano-precipitates.

The strengthening contribution from forest dislocations can be evaluated by the classic Taylor hardening model [89]:

$$\sigma_{dis} = M\alpha Gb\sqrt{\rho} \quad (9)$$

, in which M is the Taylor factor and equals to 3.06 for an FCC polycrystalline matrix, α is a constant of 0.35 [90] related to the interaction strength between dislocations, G is the shear modulus, b is the Burger's vector, and ρ is the dislocation density. The neutron diffraction results indicate that the dislocation density of the virgin sample is at around $6 \times 10^{13} \text{ m}^{-2}$ at both 293 K and 15 K (Fig.

8b). According to Eq. (12), the strengthening effects from initial dislocations are ~164 MPa at 293 K and ~196 MPa at 15 K.

The strengthening effect of grain boundaries (σ_{gb}) can be calculated via the Hall-Petch equation. The grain boundary strengthening effect keeps a linear relationship with the inverse square root of average grain size [91]:

$$\sigma_{gb} = \sqrt{\frac{G(T)}{G(RT)}} K_{gb} d^{-1/2} \quad (10)$$

, in which the Hall-Petch coefficient (K_{gb}) of $0.966 \text{ MPa} \cdot \text{m}^{1/2}$ was used based on Ref. [92], $G(T)$ and $G(RT)$ are the shear modulus at a given temperature and room temperature. With the average grain size of ~23.4 μm , the grain boundaries contributed ~200 MPa (293 K) and ~218 MPa (15 K) to the yield stress.

Next, we address the lattice friction stress (σ_{fi}) of the alloy at the two temperatures. Note that the classical solid-solution strengthening mechanism is limited to the conventional ductile alloy systems where the dislocation movement can be inhibited by the strain field arising from the mismatch between discrete and solvent atoms [93]. The flexibility of dislocation lines enables them to bend to overcome the energy barriers and take on low-energy configurations. However, as the notion of “one principal element” was abandoned in MCAs, the constituent atoms with different sizes can be randomly distributed among the matrix, in which each elemental atom in the alloys can act as a solute. In this scenario, the traditional “solvent” lattice does not exist and the spacing distance between each energy barrier can be decreased significantly [21,22,94]. Thus, the traditional methods of depicting lattice friction stress and solution strengthening effects are no longer suitable for the MEAs. According to Ref. [4], the MCAs can be treated as a stoichiometric compound with a fixed atomic ratio albeit disordered. Therefore, the traditional solid-solution hardening contribution can be included in the lattice friction effect, which can be more representative of the averaged lattice resistance provided by all types of constituent elements.

Recently, Varvenne et al. [22] proposed a general mechanistic solute strengthening theory (here named as the Varvenne-Luque-Curtin theory) for arbitrary MCAs, showing great success in predicting the YS of multiple HEAs and MEAs by correlating composition, temperature, and strain rate [94–96]. Different from traditional solute strengthening effects, the Varvenne-Luque-Curtin theory assumes the MCA is an effective-medium matrix having all the average properties of the alloy. Each substitutional element is treated as a solute embedded in the matrix and serves as local fluctuation. The strengthening effect then originates from the rising fluctuating interaction energies between dislocations and dense local fluctuations. To reduce the total potential energy, the dislocation adopts a wavy configuration and is locally pinned in a low-energy region. With the aid of the stress-assisted thermal activation, the trapped dislocation can escape the adjacent energy well and reach the next low-energy region along the dislocation gliding plane. This theory calculated the zero-temperature flow stress (τ_{y_0}) and fundamental zero-stress energy barrier (ΔE_b) at finite temperature (T) and finite strain-rate ($\dot{\epsilon}$) [22]:

$$\tau_{y_0} = A_t \alpha_t^{\frac{1}{3}} G \left(\frac{1+\nu}{1-\nu} \right)^{\frac{4}{3}} \left[\frac{\sum_n c_n \Delta V_n^2}{b^6} \right]^{\frac{2}{3}} \quad (11)$$

$$\Delta E_b = A_E \alpha_t^{\frac{1}{3}} G b^3 \left(\frac{1+\nu}{1-\nu} \right)^{\frac{2}{3}} \left[\frac{\sum_n c_n \Delta V_n^2}{b^6} \right]^{\frac{1}{3}} \quad (12)$$

, where $A_\tau = 0.04865[1 - (A-1)/40]$ and $A_E = 2.5785[1 - (A-1)/80]$ are two constants related to the core structure of FCC dislocations consisting of two separated partial dislocations accompanied with a correction for elastic anisotropy with the Zener anisotropy factor $A = 2C_{44}/(C_{11} - C_{12})$. $\alpha_i = 0.125$ is a dimensionless line tension parameter for FCC alloys [95]. ΔV_n is the misfit volume of a type- n element at composition (c_n) in the alloy [21]:

$$\Delta V_n = \frac{\partial V_{alloy}}{\partial c_m} - \sum_m^N c_m \frac{\partial V_{alloy}}{\partial c_m} \quad (13)$$

, in which $V_{alloy} = V_{alloy}(c_1, c_2, \dots, c_{N-1})$ is the atomic volume of the alloy and $\partial V_{alloy}/\partial c_N = 0$. Therefore, the volume misfit can then be experimentally determined by measuring the lattice parameter evolution over a series of alloys [95]. With the first-principles calculation, it can also be computed precisely after multiple times of replacing one type- n atom with a type- m atom at many different atomic environments [97]. In our case, we applied Vegard's law ($V_{alloy} = \sum_n c_n V_n$) to estimate the misfit volume [21,22]:

$$\Delta V_n = V_n - V_{alloy} \quad (14)$$

, where V_n is the apparent volume of the type- n element. Based on the experimental results on Ni, Ni-Cr, and Ni-Fe binary alloys from Ref. [22], the apparent atomic volumes of the three constituent elements Fe, Cr, and Ni were adapted to be 12.09 \AA^3 , 12.27 \AA^3 , and 10.94 \AA^3 , respectively.

At finite temperature T and finite strain-rate, Eq. (14) and (15) can be combined based on the standard thermal activation [98]:

$$\tau_y(T, \dot{\epsilon}) = \tau_{y_0} \exp\left(-\frac{1}{0.51} \frac{k_B T}{\Delta E_b(T)} \ln \frac{\dot{\epsilon}_0}{\dot{\epsilon}}\right) \quad (15)$$

, where the strain rate ($\dot{\epsilon}$) of $8 \times 10^{-5} \text{ s}^{-1}$ was used in the present study, $\dot{\epsilon}_0$ is a reference strain rate and a value of 10^4 s^{-1} was adapted according to Refs. [22,95], k_B is the Boltzmann constant. Therefore, the uniaxial friction stress can then be calculated by multiplying the shear stress by the Taylor factor:

$$\sigma_{fr}(T, \dot{\epsilon}) = M \tau_y(T, \dot{\epsilon}) \quad (16)$$

Finally, with inputs obtained from the experiments (Table 4 and 5), the lattice friction stress of the FeCrNi alloy was determined to be 316 MPa and 629 MPa at 293 K and 15 K, respectively.

According to Eq. (11), the YS of the alloy at 293 K and 15 K can be estimated to be 680 MPa and 1043 MPa, respectively. As compared in Table 5, the modeled strength shows acceptable agreement with the measured results at both temperatures. The mechanistic theory of the YS prediction of random MCAs plays a critical role in understanding the strengthening mechanisms and serves as a guideline in designing and optimizing new MCAs.

Table 5 The modeled and measured strength of the alloy at different temperatures

	293 K	15 K
σ_{dis} [MPa]	164	196
σ_{gb} [MPa]	200	218
σ_{fr} [MPa]	316	629
modeled σ_{YS} [MPa]	680	1043
measured σ_{YS} [MPa]	651±12	1092±22

4.2 Plastic deformation

According to the diffraction results (very low level of SFP (Fig. 8a), high SFE, and no phase transformation during deformation), together with the TEM observations (Fig. 10), the dislocation multiplication is the main strengthening resource and carrier of plasticity during plastic deformation. No deformation-induced twinning and phase transformation was observed during the plastic deformation. Hence, the constitutive model to depict the total flow stress (σ) of the alloy can be derived as follows:

$$\sigma = \sigma_{fr} + \sigma_{gb} + \sigma_{dis} \quad (17)$$

The strengthening effect from dislocation can be determined by Eq. (12) and the dislocation density evolution shown in Fig. 8c. After yielding, the dislocation density increased almost linearly with the true stress at both temperatures. When deforming at 293 K to a true strain of 0.31, strengthening contribution from dislocations can reach 854 MPa. At 15 K, dislocations contributed 697 MPa at a true strain of 0.12. The accumulated strengthening contributions from different resources at 293 and 15 K are compared with the measured flow stress at 293 K and 15 K as shown in Fig. 11a and 11b respectively. The model calculations agree very well with the experimental results.

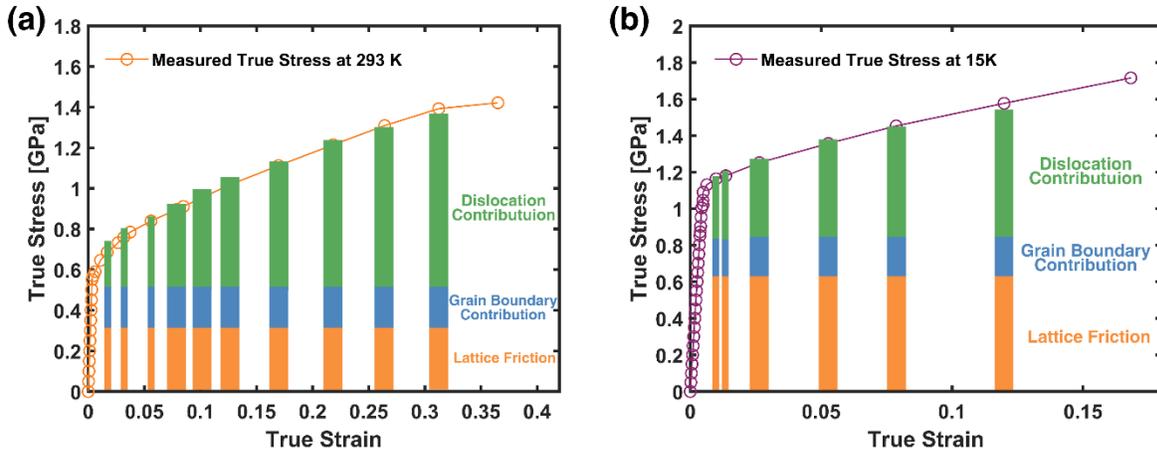


Fig. 11 The comparison between the calculated strength originating from different strengthening resources and the measured total flow stress at (a) 293 K and (b) 15 K.

Generally, the large elongation of FCC alloys can be achieved via introducing extra strengthening mechanisms (such as TWIP and TRIP effects) [13,28]. The FeCrNi has high SFE and no TWIP and TRIP effects were observed when deformed. The high SFE of the MEA means that the

activation of multiple strengthening mechanisms is impeded. Hence, the dislocation activity becomes the main strain contributor during the plastic deformation [14,28,74]. Even with only the dislocation strengthening for the FeCrNi, a notably good combination of strength and ductility was obtained. The large ductility (0.48) at 293 K might be resulted from divisive slip systems and the high dislocation multiplication capacity of the alloy. According to Ref. [99], dislocation multiplication not only can provide a significant dislocation forest hardening effect but also serves as a critical contributor to ductility improvement. As we discussed in Section 3.5, the development of texture and grain rotation favorably occurred at 293 K, promoting the activation of more slip systems at grains with a variety of orientations. This process can sustainably support dislocation multiplication, providing higher dislocation strengthening effect and improved ductility. However, the ductility deteriorated at 15 K. At 15 K, grain rotation was impeded, thus limiting the dislocation multiplication in not-so-good-orientated grains. The severe dislocation tangling phenomenon (Fig. 9) at 15 K even further reduced the ductility.

5. Conclusions

In this study, we investigated the deformation behaviors and strengthening mechanisms of an equiatomic ternary FeNiCr MEA at 293 K and 15 K. Experiments (e.g., *in situ* neutron diffraction, and post-mortem microscopy characterizations) and theoretical simulations (DFT and dislocation slip system driven modeling) were synergistically employed to map the microstructure evolution (e.g., lattice strain, SFP, shear bands, and dislocation density), determine key mechanistic parameters (single crystal elastic constants and SFE) and confirm the strengthening mechanisms. The investigation leads to the following conclusions:

1. The equiatomic ternary FeNiCr alloy showed excellent strength-ductility balance at 293 K with YS of 651 ± 12 MPa, UTS of 1020 ± 3 MPa, and total elongation of 0.48 ± 0.05 . At 15 K, ultrahigh YS of 1092 ± 22 MPa and UTS of 1451 ± 2 MPa were achieved, while the elongation decreased to 0.18 ± 0.01 .
2. MC simulation predicts the formation of short-range ordering and Fe₂CrNi intermetallic. However, no short-range orderings were observed according to the neutron diffraction spectra, APT results, and TEM analysis. This indicates the alloy is in a metastable state and the SRO effect is absent due to the sample fabrication technique used.
3. Single-crystal elastic constants and bulk elastic moduli were calculated from the neutron diffraction data, which agree well with the DFT-simulated results for the disordered configuration generated by MC simulations at 2000 K, but less well with the ordered configuration generated by MC simulation at 300 K. This again suggests that the alloy produced is in a metastable configuration.
3. At both 293 K and 15 K, the FeNiCr MEA showed high phase stability and maintained as an FCC solid solution during deformation. Meanwhile, it showed a very low level of stacking fault probability during deformation and has high SFE (63 ± 4 mJm⁻² at 293 K and 47 ± 3 mJm⁻² 15 K), indicating its inability of producing massive stacking faults and introducing TWIP and TRIP effects. The *in situ* neutron diffraction data and TEM analysis confirmed that no TWIP and TRIP effects occurred when the alloy was deformed at both temperatures.
4. The high solute misfit volumes of the FeNiCr can effectively introduce severe lattice distortion, which substantially improves the strength, especially at extremely low-temperature conditions. Based on the Varenne-Luque-Curtin theory, the strengthening contribution from the lattice distortion was calculated. At 293 K, the friction stress, resulting from the lattice distortion, can contribute 316 MPa to the YS, while it increased significantly to 629 MPa at 15 K.

5. During plastic deformation, dislocation motion and multiplication serve as the dominant deformation mechanism and the main strain carrier at 293 K and 15 K. The as-fabricated samples had a low dislocation density of $\sim 6 \times 10^{13} \text{ m}^{-2}$. After yielding, dislocation density increased almost linearly with true stress.

CRedit authorship contribution statement

L. Tang: Data curation, Formal analysis, Visualization, Writing – original draft, Writing - review & editing. **F.Q. Jiang:** TEM characterization, Writing – review & editing. **J.S. Wróbel:** DFT modeling, Writing – review & editing. **B. Liu:** Sample fabrication, Data curation, Writing – review & editing. **Saurabh Kabra:** neutron diffraction and tensile testing, Writing – review & editing. **R.X. Duan:** SEM characterization, Writing – review & editing. **Z.B. Luan:** APT characterization, Writing – review & editing. **Z.B. Jiao:** APT characterization, Writing – review & editing. **Y. Liu:** Sample fabrication, Writing – review & editing. **M.M. Attallah:** Supervision, Writing – review & editing. **D. Nguyen:** DFT modeling, Writing – review & editing. **B. Cai:** Supervision, Conceptualization, Methodology, Formal analysis, Writing- Reviewing & Editing.

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