



## Full length article

# An assessment of the lattice strain in the CrMnFeCoNi high-entropy alloy



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## ABSTRACT

The formation of single phase solid solutions from combinations of multiple principal elements, with differing atomic radii, has led to the suggestion that the lattices of high-entropy alloys (HEAs) must be severely distorted. To assess this hypothesis, total scattering measurements using neutron radiation have been performed on the CrMnFeCoNi alloy and compared with similar data from five compositionally simpler materials within the same system. The Bragg diffraction patterns from all of the studied materials were similar, consistent with a face-centered cubic structure, and none showed the pronounced dampening that would be expected from a highly distorted lattice. A more detailed evaluation of the local lattice strain was made by considering the first six coordination shells in the pair distribution functions (PDF), obtained from the total scattering data. Across this range, the HEA exhibited the broadest PDF peaks but these widths were not disproportionately larger than those of the simpler alloys. In addition, of all the materials considered, the HEA was at the highest homologous temperature, and hence the thermal vibrations of the atoms would be greatest. Consequently, the level of local lattice strain required to rationalise a given PDF peak width would be reduced. As a result, the data presented in this study do not indicate that the local lattice strain in the equiatomic CrMnFeCoNi HEA is anomalously large.

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## 1. Introduction

High-Entropy Alloys (HEAs) differ from conventional metallic materials in that they are based upon multiple atomic species in near equiatomic ratios, rather than a single principal element. It might be expected that the microstructures of these alloys would contain several intermetallic phases, but much of the literature associated with these materials has reported only solid solutions with simple crystal structures, such as face- or body-centered cubic (fcc and bcc respectively) and their related superlattice structures [1,2]. These observations have given rise to the concept of entropic stabilisation, which suggests that the configurational entropy of these multi-component solid solutions can overcome the enthalpy of formation of competing intermetallic phases [1]. However, whilst initially appealing, caution should be exercised as several

datasets have been obtained from as-fabricated material, which is likely to have been in a metastable state, as opposed to the thermodynamic equilibrium achieved by homogenisation and long duration thermal exposures [1–7]. In addition, studies using higher-resolution techniques have also revealed the presence of nano-scale precipitates in some alloys [8,9].

Nevertheless, the formation of statistically disordered single phase multi-component solid solutions is interesting, as the arrangement of the different atomic species will be far more complex than in a conventional dilute alloy. For example, in a relatively simple austenitic stainless steel, such as Fe–18Cr–8Ni wt.%, almost 75% of the atoms surrounding any given lattice site would be Fe. Conversely, in a five-component equiatomic HEA that also adopts an fcc structure, only 20% of the nearest neighbours would be atoms of the same species. This complicated arrangement of multiple atom types, each with a different size and electronic structure, is directly related to two of the four proposed HEA core effects; sluggish diffusion and severely distorted lattices [2,10,11]. Limited evidence exists for either of these effects, but data relating

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to the lattice distortion in the literature is particularly sparse and hence forms the basis of the current work [12].

It is well established that the addition of alloying elements into a pure metal causes local distortions in the regular atomic array, moving neighbouring host atoms away from their ideal positions. The strain fields associated with these distortions impede gliding dislocations, giving rise to strengthening. These concepts have been extended to the multi-component HEAs, where it has been suggested that the cumulative effect of a significant number of different atom types within the first coordination shell would generate a highly strained structure [2]. Such severely distorted arrays could give rise to a significant level of solid solution strengthening, as has been reported in a number of HEA systems [3,13–15]. However, strength could also have been influenced by the presence of nano-scale precipitates within the material and significant levels of strain would be expected to destabilise the lattice, resulting in precipitation or amorphisation [16–18]. Thus, there is an obvious need to obtain new data that can clarify this matter.

One reason for the lack of clear experimental data that elucidates the extent of the lattice distortions in HEAs is the difficulty in making suitable measurements. High-resolution transmission electron microscopy imaging of the atomic columns can show local distortions [19]. However, images of this type display an average of the signal along each atom column and are susceptible to distortions caused by other effects, such as damage caused during ion beam thinning. In diffraction experiments, the displacement of atoms away from their ideal positions would affect the observed peak intensities, in a similar manner to thermal vibrations [20,21]. Larger distortions would reduce the intensity of each diffraction peak, with that signal becoming redistributed into diffuse scattering. Several publications have presented data showing this effect [2,3,11,13,15,22,23], but the most comprehensive example is Fig. 11 in Ref. [11], which presents a series of single phase, fcc alloys with systematically increasing chemical complexity. However, lattice distortions are not the only factor that can cause a reduction in the observed peak intensity, particularly when comparing different samples measured on a laboratory diffractometer. Factors such as crystallographic texture (or lack of powder average statistics), the fluorescence of certain atomic species when irradiated by particular incident photons, and other instrumental effects would all influence the intensity of a diffraction peak. Thus, without accounting for these effects, it cannot be conclusively determined whether the atomic arrays in single phase multi-component solid solutions are severely distorted.

Recently, it has been suggested that the use of total scattering data can provide more information on the nature of the local arrangements and positions of the atoms in HEAs [24–26]. Total scattering is an extension of traditional powder diffraction measurements, wherein both Bragg and diffuse scattering are measured and analysed simultaneously. The Fourier transform of total scattering data produces a pair distribution function (PDF), which is a weighted histogram of the interatomic distances within the irradiated volume. The position and shape of the peaks in a PDF provide information on the local environment surrounding each atom, as opposed to the average structural information contained within the Bragg data. Total scattering measurements have been made on a ZrNbHf ternary alloy and an  $\text{Al}_{1.3}\text{CoCrCuFeNi}$  HEA using both X-ray and neutron radiation [24–26]. These studies have identified that the shape of the PDF peaks at short interatomic distance varied from those expected from an ideal structure and these differences were attributed to the presence of local distortions in the lattice. However, in both cases, the samples were measured in the as-cast condition, which is likely to contain solidification induced micro-segregation that could affect the PDF peak shape. Similarly, the

pronounced crystallographic texture displayed in the ZrNbHf sample and the complex three-phase microstructure of the  $\text{Al}_{1.3}\text{CoCrCuFeNi}$  HEA, would need to be accounted for, to provide an in depth understanding of the strain in these alloys [27]. Therefore, whilst these studies clearly illustrate the capability of the technique, further measurements, with careful consideration of sample complexity and condition, are required to provide a clear picture of the local environment in HEAs.

To address this issue, here we present total scattering measurements made with neutron radiation on a five-component equiatomic powder HEA sample in a single-phase condition. The sample was gas atomised to ensure that good powder diffraction data could be obtained and textural effects avoided [27]. The results are compared to data for a Ni powder, three Ni-Cr binary alloys and a Ni-Co-Cr ternary alloy. Whilst the results indicate that the strain in the HEA lattice is greater than that of pure Ni, the magnitude of this strain was similar to that observed in some of the binary and ternary alloys and cannot be considered anomalously large. As such, the data reported here do not support the overarching concept that all multi-component solid solutions must have severely distorted lattices.

## 2. Experimental methods

Gas atomised powders of Ni-33Cr (at.%) and an equiatomic CrMnFeCoNi HEA were produced by Hauner Metallische Werkstoffe. A small quantity of each powder was encapsulated within an evacuated and Ar backfilled quartz tube prior to heat treatment at 1200 °C for 2 h followed by water quenching. The heat treatment served to both chemically homogenise the material and sinter the powders into a bar. The surfaces of the sintered bars were lightly ground to remove any potential contamination from the heat treatment process.

Total scattering measurements were performed on the Polaris instrument at the ISIS Neutron and Muon Source (RB1520332 (December 2015)). To ensure that data of sufficient quality were acquired, these measurements were made for a total of 4 h under ambient conditions. The scattering data were focussed using the Mantis software [28], which corrected, normalised and collated the information from the 3008 detectors. Rietveld refinement of the Bragg data was performed using the GSAS program [29]. The total scattering data were processed using the GudrunN software [30] and Fourier transformed to obtain pair distribution functions using the SToG program, distributed as part of the RMCProfile package [31], with a  $Q_{\text{max}} = 31 \text{ \AA}^{-1}$ . Modelling of the total scattering data was also performed using the RMCProfile program.

The data collected were compared to data gathered previously under the same conditions on the Polaris instrument for Ni, Ni-20Cr, Ni-25Cr (RB1510579 (May 2015)) and Ni-37.5Co-25Cr (RB1310308 (May 2014)). The Ni was investigated in the as-received powder form, whilst the alloy specimens were all fabricated using the same method as described above but with different heat treatment parameters. The Ni-Cr binaries were heat treated for 100 h at 1000 °C, whilst the Ni-37.5Co-25Cr alloy was exposed for 100 h at 900 °C. In addition, the sintered Ni-37.5Co-25Cr alloy bar was crushed using a hand percussion mill prior to the scattering measurement. All of the data from previous experiments were reanalysed together with that from the current experiment to ensure consistency of data handling.

## 3. Results

The neutron diffraction patterns from the different alloys are shown in Fig. 1. The raw data underwent standard normalisation against pure vanadium to account for the incident neutron flux on

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