1916
doi:10.1017/S1431927619010316
Microsc. Microanal. 25 (Suppl 2), 2019

Characterisation of Misfit Dislocations at Semicoherent Interfaces in Biphasic Functional Heusler Intermetallics

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The large class of Heusler intermetallics features an array of interesting functional properties, including coupling between magnetic, structural, and electronic properties [1]. Rather than externally applied strain, strain fields can be built in to these systems through phase separation between the full Heusler (*fH, XY_2Z*) phase and the half Heusler (*hH, XYZ*) phase. Biphasic Heuslers exhibit complex microstructures, which can be tailored to control precipitate shape, size, and volume fraction, ultimately affecting the physical properties of the composite [2,3].

The present work focuses on the Nb–Co–Sn system, where $NbCo_{1.1}Sn$ was synthesized using levitation melting and subsequent annealing [4]. The scanning transmission electron micrograph (STEM) in Figure 1a shows the two-phase microstructure, which displays $NbCo_2Sn$ precipitates (*fH* phase) embedded in a NbCoSn matrix (*hH* phase). STEM assessment along a [111] zone axis reveals that the precipitates have a globular shape with no apparent matrix/precipitate interface orientation relationship. In fact, there are large regions where both phases appear to overlap; the non-overlapping parts are encircled with dotted lines. Enlarging the region marked by a red dotted square and shown in Figure 1b reveals a regular arranged dot pattern with a threefold symmetry. Figure 1c presents the [111] zone axis of the sample in a selected area diffraction (SAD) pattern. Close inspection of one of the six <220> diffraction spots shows an extra spot, providing clear experimental evidence for a lattice mismatch between the *fH* and *hH* phases. Measurement of the *fH*/*hH* spot separation distance gives a lattice mismatch of 3.3%, in good agreement with powder X-ray diffraction. Furthermore, the diffraction pattern shows no indication of a rotation or twist between the two phases, indicating that the lattices of the two phases share a common orientation. The dot pattern contrast shown in Figure 1b can be identified as a Moiré pattern, arising from equally oriented overlapping phases with different lattice parameters. A Moiré-pattern spacing $D_{M<220}$ can be determined based on the spacing of the <220> lattice planes $d^{fH}_{<220>}$ and $d^{hH}_{<220>}$, Equation 1:

$$D_{M<220>} = \frac{d^{fH}_{<220>} \cdot d^{hH}_{<220>}}{\left| d^{fH}_{<220>} - d^{hH}_{<220>} \right|} = 6.5\ nm \quad [1]$$

The 6.7 nm distance between the dark spots in Figure 1b can be attributed to the resulting Moiré pattern. Figure 2 shows the *fH*/*hH*-interface edge-on in a sufficiently thin part of the specimen amenable to high-resolution STEM imaging, which reveals a regular pattern with dark and light regions. Geometric phase analysis (GPA) was applied to analyze these putative interface dislocations. The GPA map on the right of Figure 2 shows a pattern interpreted as dislocation pairs which line up along the interface with nanometer separation. This observation corroborates interpretation of the Moiré-pattern shown in Figure 1 as a regular array of dislocations, as was recently postulated for two-layer graphene in reference [5]. These results contribute to a better understanding of the physical nature of a *fH*/*hH*-semi-coherent interface in a two-phase system with 3.3% lattice misfit. Further work is underway to clarify how this feature is affected

and how it can be controlled by different heat treatments, and how this interface structure could be tailored to influence functional properties such as magnetic structure.

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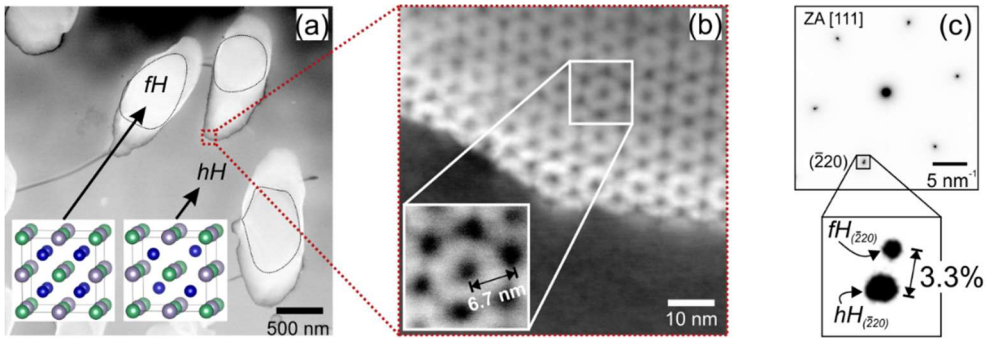

Figure 1. Two phase microstructure and corresponding diffraction data. (a) STEM micgrograph of two phase microstructure. (b) Dot pattern with three fold symmetry. (c) Documentation of [111] foil normal / zone axis. For details see text.

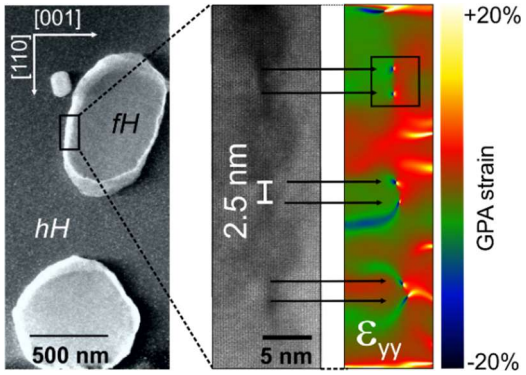

Figure 2. *fH/hH*-interface edge on. Left: Low mag STEM image of *fH*-precipitates in *hH*-matrix. Middle: High resolution image of an interface. Right: Image of local strains reveal that pairs of dislocations line up along interface. For details see text.

https://doi.org/10.1017/S1431927619010316 Published online by Cambridge University Press