Search for Significant Short-Range Ordering in Medium-Entropy Alloys

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The short-range ordering (SRO) phenomenon is a classical issue in the field of metals and alloys, such as Cu-Ni and Cu-Pd, and is once again in the spotlight, especially in high-entropy alloys. Recently, leading scientific journals have considered SRO to be a key factor in achieving a good balance between strength and toughness or ductility. However, these reports lack significant evidence linking SRO to these properties [1]. Therefore, it is necessary to quantify SRO to reveal the true relationship between SRO and the mechanical and alloy properties. The goal of SRO research is to evaluate the degree of SRO and to develop a methodology for evaluating SRO parameters using experimental techniques. To address this challenge, our recent research [2-4] aims to evaluate the Warran-Cowley SRO parameters using neutron scattering (pair distribution function) data and real-space structure modeling.

Figure 1 (left) shows the reduced pair distribution function data of the quenched Mn-Co-Ni medium-entropy alloy. For a fully random FCC structure, the height of $G(r)$ at the 1st and 2nd neighbor positions should be almost 2:1 because of the difference in coordination numbers at these positions. A similar height of $G(r)$ at these positions may indicate the existence of concentration modulation in an atom-scale region. To evaluate possible types of atom pair segregation, we attempted to determine WC-SRO parameters from our superstructure model, which was constructed using the reverse Monte Carlo method. The evaluated WC-SRO parameters are shown in Fig. 1 (right). At the nearest neighbor (N.N.) positions, the Mn-Ni atom pair is favored, while Mn-Mn and Ni-Ni pairs are favored at the next-nearest neighbor (N.N.N.) sites. The qualitative features of SRO in Mn-Co-Ni seem to be consistent with the theoretical estimations [5]. In this workshop, we will also discuss the results for other medium-entropy alloys, such as the prominent Cr-Co-Ni alloy.

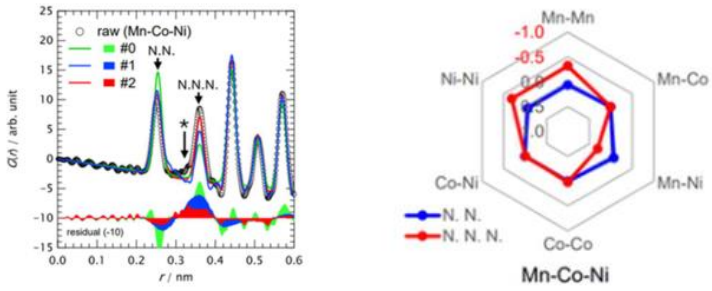

Fig. 1 Evaluated SRO parameters of Mn-Co-Ni (All data were cited from ref. 2).

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[1] R. Zhang et al., Nature **581**, 283 (2020); Note that a part of the report is later challenged by negative findings reported subsequently, as is frequently observed in such papers. [2] S. Futami *et al.*, Mater. Trans. **65**, 995 (2024). [3] Y. Ikeda *et al.*, Mater. Trans. **64**, 2254 (2023). [4] Y. Umemoto *et al.*, Mater. Trans. **64**, 2018 (2023). [5]] M. Mizuno *et al.*, Phys. Rev. Mater. **8**, 013601 (2024).