Valence Electron Concentration Dependency in Semi-Ordered High-Entropy Alloys: $L1_2$, $D0_{23}$, and $D0_{22}$ Phases

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High-entropy alloys (HEAs) with ordered-disordered coexisting structures, such as $L1_2$ and $D0_{22}$, have been reported.[1] However, the presence of longer periodic structures, represented by $D0_{23}$, has not been confirmed. In this study, we applied first-principles calculations to determine the formation energies of 15 kinds of equiatomic quaternary alloys,[2] selected from Al, Fe, Co, Ni, Cu, and Zn, as well as non-equiatomic CrFeCoNi alloys [3] with varying composition ratios of the remaining constituent elements (Fe, Co, Ni), excluding the element forming the semi-ordered phase (Cr). We then determined the conditions for the existence of ordered-disordered coexisting structures. Both equiatomic quaternary alloys and CrFeCoNi non-equiatomic alloys showed a tendency for decreasing formation energy and increasing stability in the order of $L1_2$, $D0_{23}$, and $D0_{22}$ as the value of Valence Electron Concentration (VEC) increased. These computational results provide insights into the regularity present in FCC high-entropy alloys.

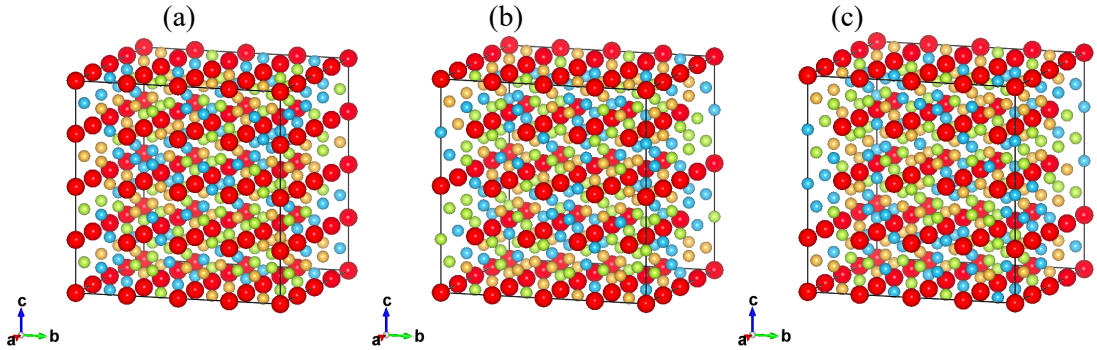

Fig.1. Crystal structures of semi-ordered (a) $L1_2$, (b) $D0_{22}$, and (c) $D0_{23}$ for quaternary alloys

References

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2. Mizuseki, H.; Sahara, R.; and Hongo, K. in preparation.
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