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Interpreting the Simplified Multicomponent Short-Range Order Parameter

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In this work we discuss the interpretation of the simplified multicomponent short-range order parameter. Crystallography is used to describe the arrangement of atoms. It is particularly powerful for most metallic materials, where the bulk can be completely defined by considering its unit cell. However, for other types of metals that lack structural long-range order (bulk metallic glass), and/or chemical long-range order (high entropy alloys), information regarding their atomic arrangement is more difficult to obtain. The short-range order (SRO) parameter is a concept introduced to extend crystallography past the unit cell, allowing for SRO characterization of disordered solutions.

The SRO parameter has been a topic of ongoing development. The Warren-Cowley short-range order (WC-SRO) parameter was introduced in 1950 to investigate binary solutions [1]; advancements have seen the parameter extended to multicomponent solutions through the pairwise [2] and generalized [3] multicomponent short-range order (PM-SRO, GM-SRO) parameters. However, the GM-SRO does not allow for consistent interpretation across all parameters. The simplified multicomponent short-range order (SM-SRO) parameter [4] was introduced to address this shortcoming.

Atom Probe Microscopy currently provides the finest resolution of any method to explore material structure at the atomic-scale. However, state-of-the-art microscopy techniques such as atom probe do not yet have the resolution required to accurately measure chemical SRO. The SM-SRO is a set of parameters that together provide a holistic description of the chemical architecture within a multicomponent solution at an atomic length scale. Additionally, it can be used to investigate atomic-scale structure in both amorphous and crystalline materials.

The SM-SRO measures solid solution architecture by two components per parameter: the sign (γ_{AB}^{m}) and the log-magnitude (λ_{AB}^{m}). There is one parameter for each reference atom and nearest neighbor (NN) atom type combination. The sign indicates the type of relationship between the reference and NN atoms: positive for segregation, negative for anti-segregation. The log-magnitude indicates the relationship strength, typically ranging from 0 to 6, where a lower number indicates a stronger relationship and 6 or higher is random.

A previously published data-set, Al -19Ag -1.67Cu (wt %) [5] was used to demonstrate the utility of the SM-SRO. The resulting SM-SRO measurements are displayed in Figure 1. A complete, holistic description of all chemical SRO in the solution is obtained as all elements are considered as both the NN and reference atom types. The sign and log-magnitude of each parameter places it along an inferred sliding scale between completely segregated, and completely anti-segregated extremes.

The power of the SM-SRO rests in its ability to reduce the chemical complexity of a multicomponent system in three-dimensional space with elemental identity, to a set of parameters along a two-dimensional area. Furthermore, the introduction of the kNN-based shell definition lends the SM-SRO to amorphous

data-sets. Although difficult to obtain, information regarding the apparently disordered micro-structure will undoubtedly progress the practicality of materials such as bulk metallic glass and high entropy alloys.

References:

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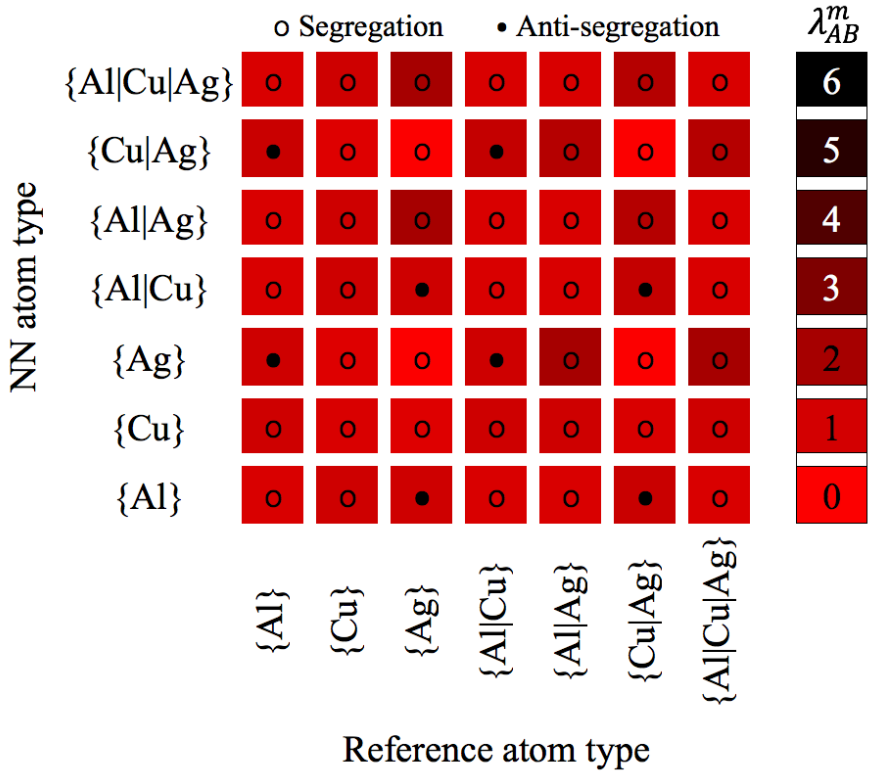

Figure 1. SM-SRO results showing interactions between sets of elements in a heat-treated Al -19Ag - 1.67Cu (wt %) alloy.