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Statistical Analysis Tools for the Local Electrode Atom Probe

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The large volumes of three dimensional information generated by the Local Electrode Atom Probe (LEAP) offer significant opportunities and challenges in the area of statistical analysis. These methods will provide valuable new insight into nanostructures occurring in the early stages of material preparation. An understanding of the transformation paths these features provide for the formation of larger precipitates and distinct phases will be fundamental in the design of new alloys with specific macroscopic properties.

Recent efforts have been directed towards qualitative and quantitative measures of co-/anti-segregation in materials. Contingency table methods are a relatively simple yet effective tool to test for the existence of correlations in the occurrences of two dilute solute species in an alloy. Contingency table analysis is an established test for departure from randomness in materials research and across many other fields[1,2], however, applying these techniques to data acquired from the LEAP requires extreme care. For example, when dissecting the data into individual blocks, not only must the number of ions be considered, but the geometric space each block occupies must also be taken into account. Blocks too anisotropic in nature can make spurious contributions to the table and should be eliminated from analysis. Further, it is fundamental to such analysis to be able make direct comparisons between two or more differently prepared samples, with a view to finding correlations with these results and the macroscopic properties exhibited by each specimen. It is known that sample size will affect contingency table χ^2 analysis (Fig. 1). This influence is further exacerbated by the tremendous amount of data generated by the LEAP and the large disparities in size that can occur between separate experiments.

Protocols are presented for the implementation of contingency table analysis and the interpretation and comparisons of subsequent findings, including the utilization of the coefficient of contingency, μ,[1,3], (Fig. 1), and the introduction of random labeling techniques to quantify results. Also presented is a density based analysis procedure, a beneficial consequence of the geometric isotropy analysis of the partitioning of the atom probe data for contingency table testing (Fig. 2).

References

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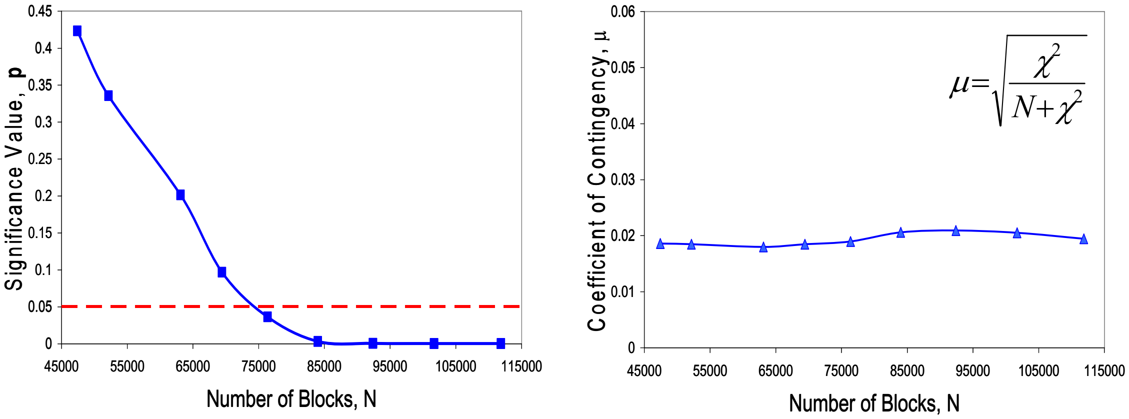

Fig. 1. Contingency table analysis of solutes occurring randomly through solvent. On left, significance value, p, dependence on sample size, N. Beneath dashed horizontal line reject null hypothesis that solutes are occurring randomly. On right, coefficient of contingency, constant with increasing N.

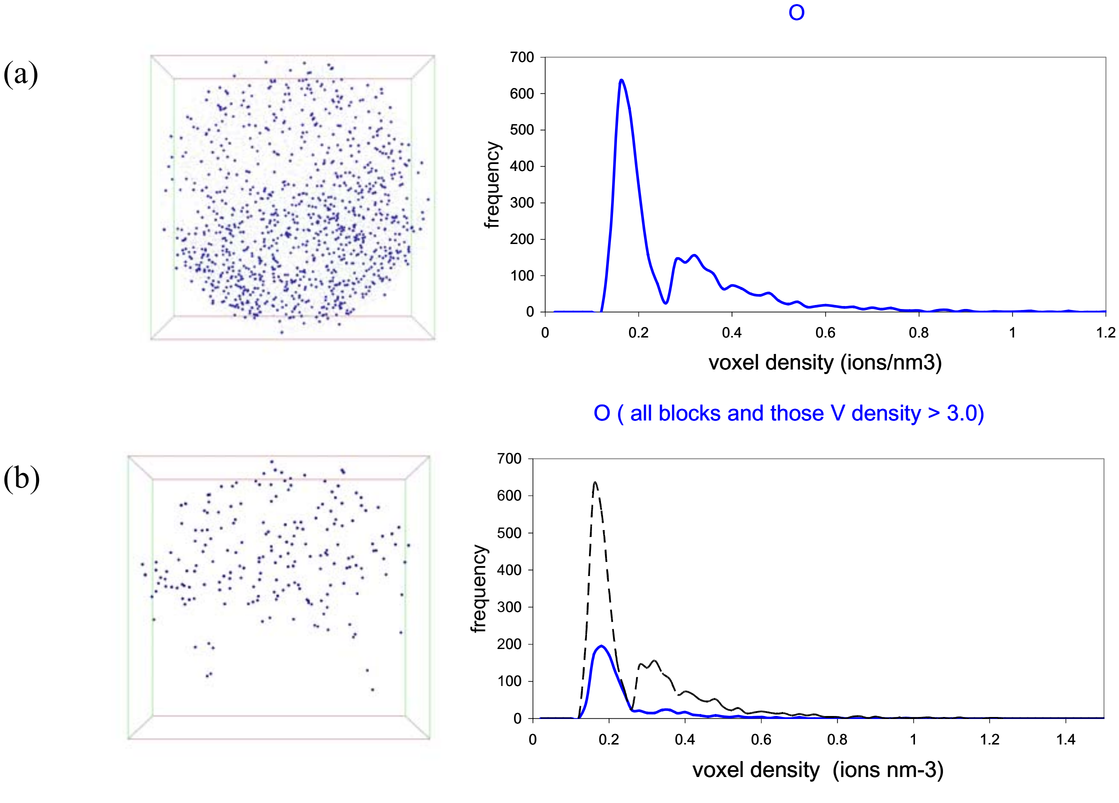

Fig. 2. (a) atom map and distribution of densities of Oxygen in multi-component Titanium alloy. (b), atom map and distributions of densities of Oxygen coinciding with regions of Vanadium density > 3.0 ions/nm^3. (Not all O atoms displayed in atom maps).