# Extracting interface correlations from the pair distribution function of composite materials

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Many important functional materials are complex mixtures that derive their properties from the interplay of various individual component phases. In each case, the *interfaces* between phases are a crucial component in their own right, since they are the point at which much of the key chemistry (and/or physics) takes place [1, 2]. By their very nature, interfaces are notoriously more difficult to characterise than the bulk phases they connect; and the process of translating experimental measurements into a picture of atomic-scale structure remains a significant general challenge [3]. Here we explore the possibility that pair distribution function (PDF) measurements offer sensitivity to interface structure in a way that is strongly complementary to existing experimental and computational approaches.

Using a non-negative matrix factorisation (NMF) approach [4, 5], we show how the PDF of complex mixtures can be deconvolved into the contributions from the individual phase components and also the interface between phases. Our focus is on the model system $Fe\|Fe_3O_4$. First, we establish proof-of-concept using idealised PDF data generated from established theory-driven models of the $Fe\|Fe_3O_4$ interface. Using X-ray PDF measurements for corroded Fe samples, and employing our newly-developed NMF analysis, we extract the experimental interface PDF ('iPDF') for this same system. We find excellent agreement between theory and experiment.
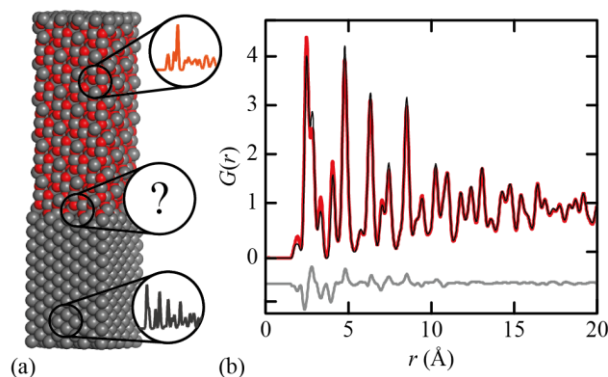


**Figure 1**. a) Representative model used to study $Fe\|Fe3O4$ interface, comprising Fe (bottom) and $Fe_3O_4$ (top); Fe atoms grey, oxygen atoms red. (b) PDFs calculated from $Fe\| Fe_3O_4$ model (red), a two-phase fit (black) using Fe and $Fe_3O_4$ PDFs, and the corresponding difference function (grey) off-set by $-0.5$ units.

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