Determination of partial structure factors in multi-component alloys

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Following Faber and Ziman [1] the determination of the partial structure factors in multi-component liquid or amorphous alloys requires $N(N+1)/2$ experimental total structure factors - which are in fact a weighted sum of the partial ones. Here, N is the number of constituents in the system under investigation. Only in the case of binary alloys - which means that three total structure factors should be measured - such an experimental study can be carried out, e.g. by means of neutron diffraction with isosopic substitution (NDIS) see [2, 3] for examples. However, not always are proper isotopes availabe and if they are, then their costs are high.

The reverse Monte Carlo modelling technique [4] provides a possibility to solve this problem. We use the example of the liquid alloys Cu_6Sn_5 [5] as well as $Ni_{33}Ge_{67}$ [6] to demonstrate that by modelling just two experimental total structure factors simultaneously, reliable partial structure factors are to be obtained for both binary alloys. These alloys have been investigated by NDIS experiments before, substituting Cu and Ni, respectively. Thus, reference data for our study is at hand. Total structure factors supplied to the simulation routine result from X-ray and neutron diffraction experiments with natural isotopic mixture in the former case, and the actual NDIS structure factors for the latter alloy.

In order to judge the influence of the amount of structural information inherent in the experimental total structure factors, a figure of merit R as proposed by McGreevy [6] has been used. This value estimates the relative information content of a number of experimental structure factors by a geometrical representation of the weight-factors relating the partial structure factors to the total ones. It showed that by increasing the structural information available to a simulation run, the differences between the NDIS partial structure factors and those obtained by RMC decrease following an approximate exponential law. This leads us to the conclusion that reliable partial structure factors can be derived by RMC modelling from less than $N(N+1)/2$ experiments provided that the relative content of structural information in the used total structure factors is high enough.

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