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**The Role of Displacement Short Range Order in the Determination of Higher Order Correlation**<sup>1</sup> YEVGENIY PUZYREV, DON NICHOLSON, MALCOLM STOCKS, GENE ICE, Oak Ridge National Laboratory — Scattering experiments are routinely used to measure pair correlation in solid solutions. Only in special cases can model structures that reproduce the pair correlation be used to determine higher order correlations. However, the requirement that measured displacement short range order also be reproduced by the model further constrains the possible higher order correlation. The determination of further restrictions on higher order correlation relies on the use of a model for atomic displacement in terms of local environment. We illustrate this procedure for a 1-d lattice-liquid using a simple displacement model and for NiFe using ab initio calculations to relate atomic displacements to local environment.

(1) Frank H. Stillinger and Salvatore Torquato, J. Phys. Chem. B 108 19589 (2004).

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