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Relationship between pair and higher order correlations in solid solutions DON NICHOLSON, ROZALIYA BARABASH, GENE ICE, CULLIE SPARKS, LEE ROBERTSON, Oak Ridge National Laboratory, CHRISTOPHER WOLVERTON, Ford Motor Co — Diffusely scattered x-rays (neutrons) are sensitive to the correlations among atomic positions. However, only pair correlations in occupation and displacement can be recovered from diffuse scattering measurements in the kinetic approximation, where as a complete description of the structure requires knowledge of higher order correlation. It has been suggested that pair correlation functions either uniquely determine the higher order correlations or that they restrict the value of higher order correlations. These issues are clarified by the presentation of simulation results and proofs that for pair potential Hamiltonians the pair correlations determine all higher order correlations and that for many body Hamiltonians they do not.

Rozaliya Barabash

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