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Reciprocal-Space Approach of Highly Inhomogeneous Systems¹ VOLODYMYR BUGAEV, Max Planck Institute for Metals Research, ALEXAN-DER UDYANSKY, Max Planck Institute for Iron Research, THOMAS DEMMER, ALEJANDRO DIAZ ORTIZ, PETER WOCHNER, HELMUT DOSCH, Max Planck Institute for Metals Research — A reciprocal-space approach for the calculation of spatial correlations in highly inhomogeneous systems is presented. Our method is based on the correlation-correction algorithm² and can also be used in the calculation of thermodynamic potentials of metallic and colloidal glasses. The interaction parameters are calculated in an iterative *k*-space (refinement) procedure that is amenable for both first-principles and semi-empirical calculations. We illustrate our approach on amorphous hard-sphere and Lennard-Jones systems.

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