The fast and natural technique for the interpolation of experimental structure factors of the melted metallic alloys

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Recently, we have proposed the PHS (Polydisperse Hard Sphere) approximation to the modeling of the interatomic correlations in metallic melts. The basis of this approximation was laid the assumptions that any metallic melt may be treated as the fluid in which the size of the constituent particles is characterized by some random hard sphere diameter distributed by a continuous distribution-function while the other intrinsic properties of these particles (e.g. masses, charges etc.) are kept constant and associated to their geometric centers.

In this work, we present regression analysis method for the modeling, analysis and filtering of the experimental data obtained by the X-ray scattering on the melts of metallic alloys. We assume any structure factor maybe presented as a polydispese hard sphere fluid which size-distribution is retrieved as the superposition of weighted two-parametric Schultz distribution functions (modes). Taking this suggestions we apply Levenberg fb- Marquardt algorithm where the regression function is the best fitted size-distribution and the estimation targets of the procedure is a set of 3N parameters (where N is number of modes which may grow dynamically during the fitting process). As the result we get the size distribution function, structure factor and radial distribution function of the modeled alloy. These three function are achieved using the analytic solution of Ornstein-Zernike equation with Percus-Yevic closures and, hence, maybe regarded as natural approximation or interpolation.

Also, the results may be used for experimental data filtering (remove non-natural deviations, some non-ideality analysis and interpolation of experimental data.