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A new approach for estimating the density of non-crystalline materials

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We propose a novel approach with which to estimate the density of liquids. The approach is based on the assumption that the systems would be structurally similar when viewed at around the length scale (inverse wavenumber) of the first peak of the structure factor, unless their thermodynamic states differ significantly. The assumption was implemented via a similarity transformation to the radial distribution function to extract the density from the structure factor of a reference state with a known density. The method was first tested using two model liquids (one is a simple liquid composed of the modified Lennard-Jones particles and the other is a molecular liquid composed of rigid tetrahedrons interacting via van der Waals forces), and could predict the densities within an error of several percent unless the state in question differed significantly from the reference state. The method was then applied to related real liquids, and satisfactory results were obtained for predicted densities. The possibility of applying the method to amorphous materials is shown, taking GeO_2 glass as an exmaple. By choosing GeO_2 at 8.5 GPa as a reference state, the method could satisfactorily reproduce the densities at higher pressures. The present method may thus pave the way for estimating density of high-density amorphous materials to which pycnometry is hardly applicable.

Biography

Takahiro Sakagami has received his Master of Science degree in Physics in 2010 from Ehime University. He has been working at AGC Techno Glass Co., Ltd since 2010. He has done his PhD course in the Department of Physics from Ehime University.

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