A Structural Model for Monatomic Liquids including Metallic Liquids

ABSTRACTS OF PAPERS
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A Structural Model for Monatomic Liquids including Metallic Liquids*

Kazuo FURUKAWA

The Research Institute for Iron, Steel and Other Metals

Abstract

Under criticism of the data of atomic radial distribution curves for eighteen monatomic liquids, a simple reduced-type structural model of liquids near their melting points having only one parameter A, which is the residual molecular diameter subtracted twice the root-mean-square amplitude of molecular vibration from the mean intermolecular distance r_1, is proposed as follows: "Let V_0 be the volume at closest packing of spherical molecules of diameter A, then the volume of liquid at T_m is 1.5 V_0 for quasi face-centred cubic lattice. But about 10 per cent of the sites in this quasi-lattice are empty, and these spaces are distributed through all interstices explaining the second peak at 1.9 r_1 of the distribution curves. Thus the total volume is about 1.65 V_0."

Combining this model with the free volume theory several molecular properties of monatomic van der Waals and metallic liquids including spherico-symmetrical molecular liquids are explained; for example, the shapes and positions of 1st and 2nd peaks in the radial distribution curves, the entropies, the self-diffusion coefficients and the viscosity coefficients at their melting points.

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