

Mathematical modeling of discontinuity in solid-liquid transition

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The molecular simulation of hard-sphere[1, 2] reveals that solid-liquid transition has discontinuity which is absent in liquid-vapor transition. Recently, Yokozeki[3] proposed a simple modified van der waals equation applicable to solid-liquid transition. However, this equation has a flaw in its repulsive contribution since this contribution has negative value, inconsistent with physical meaning of repulsive contribution. In this work, we propose a repulsive contribution which is always positive over a whole density region and capable of representing discontinuity in solid-liquid transition. The proposed contribution is derived in the framework of lattice fluid by proposing an insertion probability which contains two zero point.

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[2]. Alder, B.J. and T.E. Wainwright, Phase Transition in Elastic Disks. Physical Review, 1962. 127(2): p. 359.

[3]. Yokozeki, A., Analytical equation of state for solid-liquid-vapor phases. International Journal of Thermophysics, 2003. 24(3): p. 589-620.