

Figure 9.2. Yoshida–Kamakura potential (expressed in ϵ units), for different values of the softness parameter: $a = 5$ (black solid line), 3 (blue dashed line), 2 (green dotted line), 1 (red dash-dotted), and 0.5 (magenta dash-double-dotted line). The interparticle distance r is in σ units.

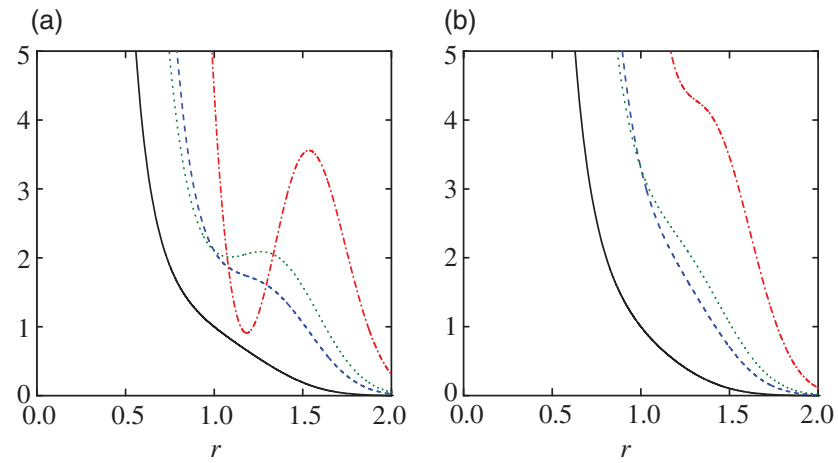


Figure 9.3. Yoshida–Kamakura potential $u(r)$ (solid line, expressed in ϵ units), two-body force $f(r) = -u'(r)$ (blue dashed line, ϵ/σ units), product $rf(r)$ (green dotted line, ϵ units), and second derivative of the potential $u''(r)$ (red dash-dotted line, ϵ/σ^2 units) for $a = 2.1$ (a) and $a = 3.3$ (b). The interparticle distance r is in σ units.

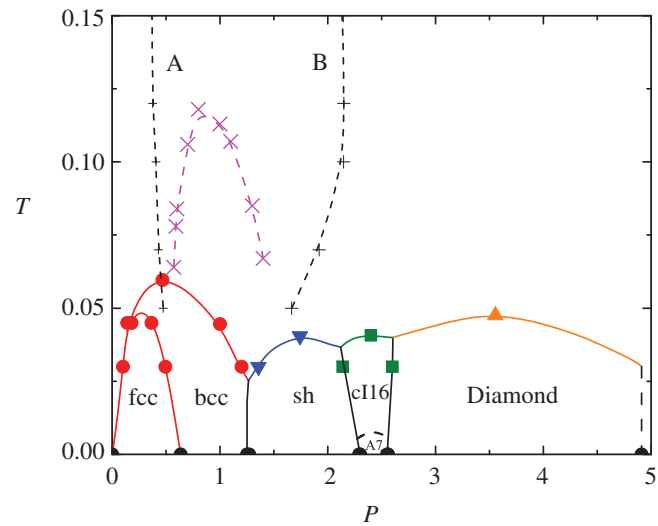


Figure 9.4. Phase diagram of the Yoshida–Kamakura interaction model for $a = 2.1$. Pressure P and temperature T are in units of ϵ/σ^3 and ϵ/k_B , respectively, k_B being Boltzmann’s constant. Full symbols are two-phase coexistence points. The data points lying on the $T = 0$ axis are exact solid–solid boundaries. The dashed line connecting crosses is the locus of density maxima in the fluid phase. Curves A and B connect points of maximum and minimum values of $-s_2$, respectively. The open region between A and B is the structurally anomalous region. Data are from Ref. [77].

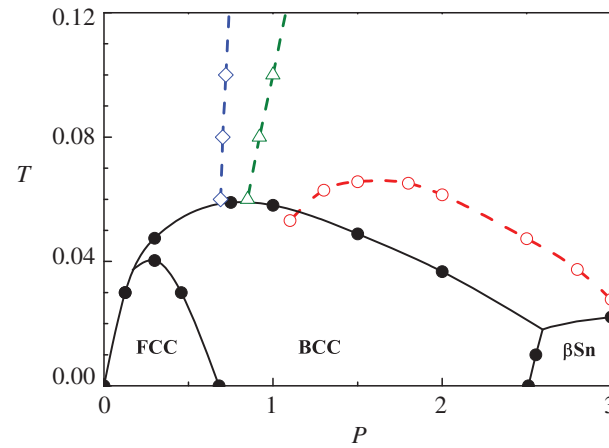


Figure 9.5. Phase diagram of the Yoshida–Kamakura potential for $a = 3.3$. P and T are in reduced units. Full dots are two-phase coexistence points. Open dots are points of density maximum in the fluid phase. Diamonds and triangles denote points of $-s_2$ maxima and D minima, respectively (D being the self-diffusion coefficient), giving the left boundary of the regions of structural and diffusion anomaly (the right boundaries, which are defined by $-s_2$ minima and D maxima, are out of the P range shown). Data are from Ref. [88].

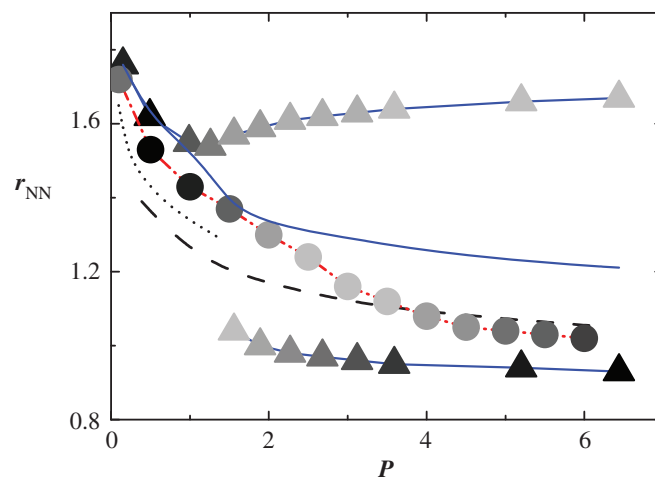


Figure 9.8. Position r_{NN} of the NN peak of $g(r)$ in units of σ as a function of P at constant T for: $u_{YK}(r)$, $a = 2.1$, and $T = 0.07$ (blue solid line and triangles); $u_{YK}(r)$, $a = 3.3$, and $T = 0.06$ (red dash-dotted line and full dots); $u_{IP}(r)$ and $T = 0.06$ (dotted line, stopping near the melting point); $u_{IP}(r)$ and $T = 1$ (dashed line). The gray scale is proportional to the height of the $g(r)$ peak. The blue line without symbols represents a weighted average of the two r_{NN} branches with weights proportional to the respective $g(r)$ peak heights, for the case $u_{YK}(r)$, with $a = 2.1$. Data are from Ref. [88].