<table>
<thead>
<tr>
<th>Title</th>
<th>Dynamic van der Waals Theory: A Phase Field Model of Fluids</th>
</tr>
</thead>
<tbody>
<tr>
<td>Author(s)</td>
<td>Omiki, Akira</td>
</tr>
<tr>
<td>Citation</td>
<td>物性研究 (2004), 83(3): 323-324</td>
</tr>
<tr>
<td>Issue Date</td>
<td>2004-12-20</td>
</tr>
<tr>
<td>URL</td>
<td><a href="http://hdl.handle.net/2433/110129">http://hdl.handle.net/2433/110129</a></td>
</tr>
<tr>
<td>Right</td>
<td></td>
</tr>
<tr>
<td>Type</td>
<td>Departmental Bulletin Paper</td>
</tr>
<tr>
<td>Textversion</td>
<td>publisher</td>
</tr>
</tbody>
</table>

Kyoto University
Dynamic van der Waals Theory
A Phase Field Model of Fluids

Kyoto Univ. Akira Onuki

In usual theories of phase transitions, the fluctuations of the temperature $T$ are assumed to be small and are neglected. However, there can be situations in which phase transitions occur in inhomogeneous $T$. For example, wetting properties near the gas-liquid critical point are very sensitive to applied heat flux and boiling processes remain largely unexplored [A. Onuki, Phase Transition Dynamics (Cambridge, 2002)]. To treat such problems we propose to start with a coarse-grained entropy rather than a Ginzburg-Landau free energy. For one-component fluids, let an entropy functional $S$ be determined by the local number density $n = n(r,t)$ and the local internal energy density $e = e(r,t)$ as

$$
S = \int dr \left[ ns - \frac{1}{2} C|\nabla n|^2 \right]
$$

We assume that $s = s(n,e)$ is the entropy per particle defined as a function of $n$ and $e$. The gradient term represents a decrease of the entropy due to inhomogeneity of $n$. We introduce the local temperature $T = T(n,e)$ by

$$
\frac{1}{T} = \frac{\delta}{\delta e} S
$$

where $n$ is fixed in the derivative. For the special form of Eq.1 we simply obtain $1/T = n(\partial s/\partial e)_n$. Maximization of $S$ under a fixed total particle number $\int dr n$ and a fixed total energy $\int dr e$ leads to the equilibrium conditions $T = \text{const.}$ and $h/T = \delta S/\delta n = \text{const.}$ As first derived by van der Waals, the equilibrium interface density profile $n = n(x)$ is determined by $h = \mu(n,T) - C T d^2 n/dx^2 = \text{const.}$ [J.S. Rowlinson, J. Stat. Phys. 20, 197 (1979)]. In the van der Waals theory $s = s(n,e)$ is given by

$$
\begin{align*}
\frac{1}{T} &= k_B \ln\left[\frac{e}{n} + \epsilon \nu \right]^{d/2} (1/\nu n - 1) \right] + \text{const.}
\end{align*}
$$

where $\nu_0$ and $\epsilon$ are positive constants representing the molecular volume and the magnitude of the attractive potential, respectively, and $d$ is the space dimensionality.

The reversible part of the stress tensor reads

$$
\Pi_{ij} = p \delta_{ij} + CT \left[ \nabla_i n \nabla_j n - (n \nabla^2 n + |\nabla n|^2/2) \delta_{ij} \right]
$$

where $p = n(\mu + s') - e$ is the van der Waals pressure. The mass density $\rho = mn$ obeys the continuity equation. The momentum density $J = \rho v$ and the energy density obey appropriate dynamic equations.
including the gradient part of the stress tensor. The entropy production rate \( dS/dt \) within the fluid is non-negative-definite if there is no heat flow from outside.

We give a numerical solution of our phase field model imposing a wetting boundary condition on all the boundaries. At \( t = 0 \) we placed a gas droplet at the center of the cell in equilibrium at \( T' = 0.875 T_c \). The bottom boundary was then increased by a constant \( \Delta T = 0.054 T_c \) for \( t > 0 \), while the top boundary was held at the initial temperature. There is no gravity, while we use "bottom" and "top". Fig.1 shows droplet migration toward the bottom, caused by a Marangoni effect. See a first report: N. O. Young et al., J. Fluid Mech. 6, 350 (1959) (where bubbles and liquid were different fluids and there was no first-order transition at the interface). Fig.2 displays the velocity and the temperature in the steady state. It is a new finding that the velocity component through the interface is nonvanishing, leading to latent heat transport. Because it is highly efficient, a flat temperature or no temperature gradient appears inside the droplet. In the steady state the gas droplet apparently wets the bottom partially, while a very thin liquid layer is sandwiched between the bottom boundary and the droplet. We can define an apparent contact angle \( \theta_{\text{eff}} \), which is a decreasing function of \( \Delta T' \). Garrabos et al. observed in space that gas spreads on a heated wall initially wetted by liquid and exhibits an apparent contact angle even larger than \( \pi/2 \) [Phys. Rev. E 64, 051602 (2001)]. With further increasing \( \Delta T' \) the heated wall is completely covered by gas, eventually leading to film boiling in gravity.