ASYMPTOTICALLY PERIODIC $L^2$ MINIMIZERS
IN STRONGLY SEGREGATING DIBLOCK COPOLYMERS

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Abstract. Using the delta correction to the standard free energy [4] in the
elastic setting with a quadratic foundation term and some parameters, we in-
troduce a one dimension only model for strong segregation in diblock copoly-
mers, whose sharp interface periodic microstructure is consistent with experi-
ment in low temperatures. The Green’s function pattern forming nonlocality
is the same as in the Ohta-Kawasaki model. Thus we complete the statement
in [31, p. 349]*: “The detailed analysis of this model will be given elsewhere.
Our preliminary results indicate that the new model exhibits periodic mini-
mizers with sharp interfaces.” We stress that the result is unexpected, as the
functional is not well posed, moreover the instabilities in $L^2$ typically occur
only along continuous nondifferentiable “hairs”.

We also improve the derivation done by van der Waals and use it and the
above to show the existence of a phase transition with Maxwell’s equal area
rule. However, this model does not predict the universal critical surface tension
exponent, conjectured to be $11/9$. Actually, the range $(1.2, 1.36)$ has been
reported in experiments [21, p. 360]. By simply taking a constant kernel, this
exponent is 2. This is the experimentally ($\pm 0.1$) verified tricritical exponent,
found e.g., at the consolute $0.9$ K point in mixtures of $^3$He and $^4$He. Thus
there is a third unseen phase at the phase transition point.

Key to some recent developments in modern microelectronics has been the ability
to create high-quality atomically abrupt interfaces between different semiconduc-
tors, which can produce new quantum states and uncover unexpected phenomena
(see http://en.wikipedia.org/wiki/Nanotechnology). Several experiments contra-
dicting common knowledge about bulk materials having only diffuse interfaces have
been reported, see the References, especially [7], where a new experimental tech-
nique is explained.

It is remarkable that chemically diverse diblock copolymers and microemulsions
admit very similar characteristic structures, e.g., the bicontinuous ordered double
diamond [27]. A theory formally predicting the phase transition between weak and
strong segregation was derived in [4]. Here we show how to use elasticity and choose
parameters in the Vaserstein pseudoassociation potential to get local $L^2$ minimizers
resembling the square wave [38]. As a by-product we get a rigorous proof of the
gas to liquid phase transition.

To make this note self-consistent, we review the history of this modeling.

The ideal gas law

$$P = \frac{RT}{V}$$

(0.1)

* A preliminary version of this result was announced at the “Defects and their dynamics”
workshop (09.08-16.08.2003), Banff International Research Station, Alberta, Canada.
where $P$ is the internal pressure, $V$ the volume per mole, $T$ the absolute temperature, $R$ the gas constant, does not predict a phase transition between gas and liquid, defined according to experiment as two densities coexisting at the same pressure (see e.g., the isotherms for carbon dioxide in [36]).

Van der Waals formulated the modified equation of state as

$$P = \frac{RT}{V - b} - \frac{a}{V^2},$$

where $a$ is the attraction parameter which arises from polarization of molecules into dipoles and $b$ is the volume enclosed within a particle (the repulsion parameter). Below the critical temperature isotherms for (0.2) have a wiggle [36], which is unphysical. Maxwell’s construction in which the fluid is taken around a reversible cycle of states from a logical point of view is worthless [36], as states on the wiggle have no meaning. However, such soft reasoning can give other interesting results [22, 36].

For uniform systems, the Helmholtz free energy is defined as $\Psi = U - TS$, where $U$ is the internal energy and $S$ is the entropy. The first law of thermodynamics states $\delta U = \delta Q - P \delta V$, where $\delta Q$ is heat change, the second law for reversible systems states $\delta Q = T \delta S$. Thus $d\Psi = dU - TdS - SdT = \delta Q - PdV - TdS - SdT$, so $P = -\frac{\partial \Psi}{\partial V}$ and $\Psi = -\int PdV$. Since the isothermal compressibility $\beta$ satisfies $\beta \equiv -\frac{1}{V} \frac{\partial V}{\partial P} \geq 0$, we get $\frac{\partial^2 \Psi}{\partial V^2} \geq 0$. From (0.2) we get

$$\Psi^{\text{unif}} = -\int PdV = -RT\ln(V - b) - \frac{a}{V},$$

and the convex envelope of (0.3) gives Maxwell’s equal area rule for the isotherms of (0.2). However, this and related statistical mechanics arguments lack a proof of phase transition as defined above. To be more precise, suppose that Maxwell’s envelope is on the line segment $[V_1, V_2]$. Why does the system take on only $V_1$ and $V_2$, but not other values inside the segment? In other words, the implicit meaning of arguing this way is that assuming there is a phase transition, it is determined by the equal area rule.

As is often the case in mathematics, we can get a proof of phase transition with Maxwell’s equal area rule by studying a related larger structure. This was done in [20, p. 40]. In a related work, the author also obtained $4/3$ as the critical exponent [21, p. 360]. Other methods have reported $3/2$ (van der Waals), 1.38 [28] and (1.21, 1.32) [42].

We now improve the derivation of van der Waals.

Let $\rho = \frac{1}{V}$ denote the density. The free energy of a nonuniform state $\rho(x)$ of a nonreversible process is a functional of the Helmholtz form $I(\rho) = U(\rho) - TS(\rho)$. The cumulative free energy $\int_0^1 \rho I^{\text{unif}}(\rho)dx$ is:

$$\Psi^{\text{nonunif}}(\rho) = \int_0^1 \rho \Psi^{\text{unif}}(\rho) = \int_0^1 [-RT\rho \ln(\rho^{-1} - b) - a\rho^2].$$

$U(\rho)$ cannot be only $\int_0^1 (C - a\rho)\rho$, but rather $\int_0^1 \int_0^1 J(x - y)\rho(x)\rho(y)dxdy \approx \int_0^1 \rho(C - a\rho - \frac{\rho''}{2}\rho'')dx$. Since the term $\int_0^1 C\rho$ can be neglected due to the mass constraint, one can conclude that

$$I(\rho) = \Psi^{\text{nonunif}}(\rho) = \int_0^1 \frac{\rho''}{2}\rho'\rho + \int_0^1 [-RT\rho \ln(\rho^{-1} - b) - a\rho^2]$$
Note that $-a\rho^2 - RT\rho(\ln(\rho^{-1} - b))$ is concave (double-well) for $\rho$ and $T$ satisfying $RT \geq (\text{<}) 2a\rho(1-\rho)^2$. However, note that the nonlocal and the $-\int_0^1 a\rho^2$ terms appeared quite separately, therefore it may not be entirely convincing that one is an extension of the other. Also, if $-\int_0^1 a\rho^2$ is replaced by $-\int_0^1 \int_0^1 J(x-y)\rho(x)\rho(y)dx\,dy$, the solutions of the EL equation are always continuous, so we have no phase transition as defined above.

In his Nobel lecture, van der Waals expressed his absolute conviction that molecules associate in complexes not of chemical origin. He called them pseudoassociations. Thus the derivation can be improved by adding the nonlocal term to (0.4):

\begin{equation}
I^{\text{mod}}(\rho) = -\int_0^1 \int_0^1 J(x-y)\rho(x)\rho(y)dx\,dy + \int_0^1 [-RT\rho(\ln(\rho^{-1} - b) - a\rho^2)].
\end{equation}

The mass constraint makes possible an addition of a linear term, which we choose so that $-RT\rho\ln(\rho^{-1} - b) - a\rho^2$ has equal depth wells. Also, on a bounded interval boundary effects may come into play, so $J$ is not necessarily translationally invariant: $J = J(x, y)$. Now (0.6) is qualitatively the same as derived in [4]

\begin{equation}
I(u) = \frac{1}{4} \int_0^1 \int_0^1 J(x,y)(u(x) - u(y))^2 dx\,dy + \int_0^1 W(u(x))dx,
\end{equation}

where $W$ is the double-well function

\begin{equation}
W(u) = -\frac{1}{2}ju^2 + \frac{1}{2}u^2 + kT[(1 + u)\ln(1 + u) + (1 - u)\ln(1 - u)],
\end{equation}

with $J(x) = \int_0^1 J(x, y)dy$ and $k$ the Boltzmann’s constant. For some works on this and related models see the References, especially the collective diffusion kinetics of the phase transition in polymer gels, what the authors in [24] consider one of the most exciting problems in current condensed matter physics, and a nonlocal in time evolution discussed in [37].

Let $G(u) = -\frac{1}{4}u^2 + kT[(1 + u)\ln(1 + u) + (1 - u)\ln(1 - u)]$, $G^*$ be the convex envelope of $G$ and

\begin{equation}
I^*(u) = -\frac{1}{2} \int_0^1 J[u](x)u(x)dx + \int_0^1 G^*(u(x))dx.
\end{equation}

Let $g^* = G^*[u, \overline{u}]$ be the interval on which $g^*$ is constant and $v^* = g^*(u) = g^*[\overline{u}, u]$. We define

\[\mathcal{A}(v) = \begin{cases}
g^{*^{-1}}(v), & v \neq v^*, \\
\overline{u}, & v = v^*,
\end{cases} \quad \mathcal{B}(v) = \begin{cases}
g^{*^{-1}}(v), & v \neq v^*, \\
\overline{u}, & v = v^*.
\end{cases}\]

Let $u$ be a local minimizer of (0.7). Let $v = g(u)$ and $x_0$ be such that $v(x_0) = v^*$. We now show that under some conditions $v'(x_0) \neq 0$, which implies that the set of discontinuities of $u$ is finite.

Let $\delta_0 > 0$ be such that $J(x, y) > \frac{1}{2}J(x, x)$ for all $(x, y)$ such that $|x - y| < 2\delta_0$. Let $\delta \in (0, \delta_0)$ and $I_\delta = [x_0 - \delta, x_0 + \delta]$. We define

\[v^+ = \delta^2 + \max\{v(x) | x \in I_\delta\}, \quad v^- = \min\{v(x) | x \in I_\delta\} - \delta^2.\]

Let

\begin{equation}
\phi = (u - \mathcal{A}(v^-))\chi_{I_\delta} - \frac{1}{1 - 2\delta} \left( \int_{I_\delta} (u - \mathcal{A}(v^-))\chi_{[0,1]\setminus I_\delta} \right).
\end{equation}
In a similar manner, we take \( \delta \) where \( v \) thus
\[
\frac{1}{2} \int_{I_{\delta}} \phi J[\phi] \geq \int_{I_{\delta}} \phi^2 - \frac{\max_{x \in I_{\delta}} j(x)}{2(1 - 2\delta)} (\int_{I_{\delta}} \phi)^2
\]
On \([0, 1] \setminus I_{\delta}\) we have
\[
G^*(u) - G^*(u - \phi) - v\phi \geq (g^*(u - \phi) - g^*(u)) \frac{-1}{1 - 2\delta} \int_{I_{\delta}} \phi
\]
and
\[
\frac{1}{2} \int_{I_{\delta}} \phi J[\phi] \geq -\frac{\max_{x \in I_{\delta}} j(x)}{(1 - 2\delta)^2} (\int_{I_{\delta}} \phi)^2 + O\left((\int_{I_{\delta}} \phi)^3\right)
\]
Taking into account these inequalities we obtain
\[
0 \geq \left\{ \frac{J(x_0, x_0)}{4} + \int_{[0, 1] \setminus I_{\delta}} \int_{[0, 1] \setminus I_{\delta}} J - \frac{\max_{x \in I_{\delta}} j(x)}{1 - 2\delta} - \frac{\int_{[0, 1] \setminus I_{\delta}} J}{(1 - 2\delta)^2} \right\} (\int_{I_{\delta}} \phi)^2 + (v^- - v^+) \int_{I_{\delta}} \phi + O\left((\int_{I_{\delta}} \phi)^3\right).
\]
Denote the expression in the curly brackets by \( C(J, g, \delta) \). After dividing by \( \int_{I_{\delta}} \phi \) we get
\[
v^+ - v^- \geq C(J, g, \delta) \int_{I_{\delta}} (u - \mathbb{H}(v^-)) + O(\delta^2).
\]
In a similar manner, we take
\[
\phi = (u - \mathbb{H}(v^+)) \chi_{I_{\delta}} - \frac{1}{1 - 2\delta} \left( \int_{I_{\delta}} (u - \mathbb{H}(v^+)) \chi_{[0, 1] \setminus I_{\delta}} \right)
\]
and obtain
\[
v^+ - v^- \geq C(J, g, \delta) \int_{I_{\delta}} (\mathbb{H}(v^+) - u) + O(\delta^2).
\]
Adding these two inequalities and dividing by \( 2\delta \) we get
\[
\frac{v^+ - v^-}{2\delta} \geq \frac{C(J, g, \delta)}{2} (\mathbb{H}(v^+) - \mathbb{H}(v^-)) + O(\delta).
\]
Letting \( \delta \to 0 \) we get
\[
|v'(x_0)| \geq \frac{C(J, g)}{2}(u - \bar{u}),
\]
where
\[
C(J, g) = \frac{J(x_0, x_0)}{4} + \frac{1}{\delta} \int_{I_{\delta}} J - j(x_0) \int_0^1 g'(u).
\]
Thus \( v'(x_0) \neq 0 \) if \( C(J, g) > 0 \). For now this shows that any local minimizer does not take values in \((\bar{u}, \bar{u})\) and proves the existence of phase transition.
The well-balanced scaling

\begin{equation}
J_\epsilon(x, y) = \frac{1}{\epsilon} J^s \left( \frac{x - y}{\epsilon} \right) - \epsilon J^l(x, y),
\end{equation}

proposed in [31], where \( J^s \geq 0 \) and \( \int_R |x| J^s(x)dx < \infty \), can be justified as representing an interplay of attractive \((J^s)\) and repulsive \((J^l)\) chemical forces. This is consistent with an established view in physical chemistry, e.g., “But the establishment of a well-defined periodicity between the lamellae, or the rods, depends on the existence of long-range forces between them: attractive (van der Waals) or repulsive (electrostatic, steric, plus the short-range Marcelja repulsion)” [12, p.2296].

Its qualitative shape of that of the “mexican hat”, a notion that comes from mathematical biology, where such kernels are also often used. However, it is interesting to observe that since we assume only \( \int_R |x| J^s(x)dx < \infty \), \( J_\epsilon \) can be nonnegative. It is then its shape, not sign, that gives pattern formation.

The construction of periodic minimizers with discontinuous interfaces now follows from a sequence of lemmas. Let \( I_\epsilon \) denote \( I \) with \( J_\epsilon \) given by (0.11). Then \( \epsilon^{-1} I_\epsilon \Gamma\)-converges as \( \epsilon \to 0 \) to a singular limit defined on \( L^2(0, 1) \) by

\[
I_0(u) = \begin{cases} 
0 & \text{if } u \in BV((0, 1), \{-1, 1\}) \\
\frac{c_0}{2} ||Du||^2(0,1) - \frac{1}{4} \int_0^1 \int_0^1 J^s(x, y)(u(x) - u(y))^2 \, dx \, dy & \text{otherwise},
\end{cases}
\]

where \( c_0 = \inf \{ ||u|| = \pm 1 \} \) \( \frac{1}{4} \int_0^1 \int_0^1 J^s(x, y)(u(x) - u(y))^2 \, dx \, dy + \int_R W(u(x)) \, dx \) and \( ||Du|| \) is the variation measure of \( u \) [1]. Here \( \Gamma \)-convergence is defined as

1. For every \( \{u_\epsilon\} \subset L^2(0, 1) \) with \( \lim_{\epsilon \to 0} u_\epsilon = u \), \( \liminf_{\epsilon \to 0} \epsilon^{-1} I_\epsilon(u_\epsilon) \geq I_0(u) \);
2. For every \( u \in L^2(0, 1) \cap BV((0, 1), \{-1, 1\}) \), there exists a family \( \{u_\epsilon\} \subset L^2(0, 1) \) such that \( \lim_{\epsilon \to 0} u_\epsilon = u \), and \( \limsup_{\epsilon \to 0} \epsilon^{-1} I_\epsilon(u_\epsilon) \leq I_0(u) \).

These two inequalities often go together the compactness property

3. Let \( \epsilon_n \) be a sequence of positive numbers converging to 0, and \( \{u_n\} \) a sequence in \( L^2(0, 1) \). If \( \epsilon_n^{-1} I_{\epsilon_n}(u_n) \) is bounded above in \( n \), then \( \{u_n\} \) is relatively compact in \( L^2(0, 1) \) and its cluster points belong to \( BV((0, 1), \{-1, 1\}) \).

A further related property is that a strict local minimum \( u_0 \) of \( I_0 \) perturbs to a local minimum \( u_\epsilon \) of \( \epsilon^{-1} I_\epsilon \). This was shown and used in [23] to obtain local minimizers on dumbbell domains. In the proof, by a standard argument, a minimizer \( u_\epsilon \) of \( \epsilon^{-1} I_\epsilon \) is first constructed in a small closed ball around \( u_0 \). Then using properties 1 – 3 it is shown that for small enough \( \epsilon > 0 \), \( u_\epsilon \) lies in the interior of the ball, thus is a local minimizer of \( \epsilon^{-1} I_\epsilon \) in \( L^2 \).

When \( G \) is nonconvex this argument goes through a convexification and the calculation above. It is shown that a local minimum of \( I_0^* \) in a subspace of \( BV((0, 1), \{-1, 1\}) \) having a fixed number of jumps is also a local minimum of \( I_0^* \) in \( L^2(0, 1) \). This observation reduces the problem of determining local minima of \( I_0^* \) to a finite dimensional one. Since \( \frac{1}{4} ||Du||(0,1) \) is equal to the number of jumps of \( u \), it is enough to investigate only the second term of \( I_0^* \). In general, its critical points are determined from a system of nonlinear algebraic equations and this is not an easy, or indeed, pleasant task.

The Ohta-Kawasaki functional follows from [2], though it has been shown in [27] that it is not sophisticated enough to predict the complicated phase separation morphologies. However, to confirm that pseudoassociations exist and to calculate the critical point exponent, we make a study in one dimension.
The robust functional

\[ I(w) = \int_0^1 \frac{1}{2} \epsilon^2 w''(x)^2 + W(w'(x)) + w^2(x) dx, \]

can model e.g., the twinned martensite phase in Nitinol [25]. The elastic foundation third term in (0.12) is nonlocal. Namely, let us consider (0.12) with the boundary conditions \( w(0) = w(1) = 0 \). Let \( w = v', \ v = (-D^2)^{-1}(u - m) \), where

\[-D^2 : \{ v \in W^{2,2} : v'(0) = v'(1) = 0, \int_0^1 v = 0 \} \rightarrow \{ w \in L^2 : \int_0^1 w = 0 \}.\]

Then \( w' = v'' = m - u, \ w'' = -u' \) and

\[ \int_0^1 u''x = \int_0^1 v'^2 = - \int_0^1 v''v = \int_0^1 (u - m)(-D^2)^{-1}(u - m) = \int_0^1 u(-D^2)^{-1}u \]

and (0.12) becomes

\[ I(u) = \int_0^1 \frac{1}{2} \epsilon^2 u'(x)^2 + W(m - u(x)) dx + \int_0^1 \int_0^1 G(x, y)u(x)u(y) dx dy, \]

with \( G \) as in [32]. Using the improved van der Waals derivation, we obtain (0.7) with \( J = J_\epsilon \) - the strong separation diblock copolymer functional. With \( G \) and small \( \epsilon \) - asymptotically periodic local minimizers with sharp interfaces.

References

[1] G. Alberti and G. Bellettini, A non-local anisotropic model for phase transitions: asymptotic behaviour of rescaled energies, European J. Appl. Math. 9 (1998), 261-284.
[2] J. M. Ball and C. Mora-Corral, A variational model allowing both smooth and sharp phase boundaries in solids, Commun. Pure Appl. Anal., in press.
[3] P. W. Bates and P. Chmaj, An integrodifferential model for phase transitions: stationary solutions in higher space dimensions, J. Statist. Phys. 95 (1999), 1119-1139.
[4] P. W. Bates, P. C. Fife, X. Ren and X. Wang, Traveling waves in a convolution model for phase transitions, Arch. Rational Mech. Anal. 138 (1997), 105-136.
[5] P. W. Bates, P. C. Fife, X. Ren and X. Wang, Traveling waves in a convolution model for phase transitions, Arch. Rational Mech. Anal. 138 (1997), 105-136.
[6] M. Bode, Spin-polarized scanning tunneling microscopy, Rep. Prog. Phys. 66 (2003), 523-582.
[7] D. Brandon and R. C. Rogers, The coercivity paradox and nonlocal ferromagnetism, Contin. Mech. Thermodyn. 4 (1992), 1-21.
[8] J. Carr and R. Pego, Invariant manifolds for metastable patterns in \( u_t = \epsilon^2 u_{xx} - f(u) \), Proc. Roy. Soc. Edinburgh Sect. A 116 (1990), 133-160.
[9] X. Chen and Y. Oshita, An application of the modular function in nonlocal variational problems, Arch. Rational Mech. Anal. 186 (2007), 109-132.
[10] R. Choksi and P. Sternberg, On the first and second variations of a nonlocal isoperimetric problem, J. Reine Angew. Math. 611 (2007), 75-108.
[11] P. G. De Gennes and C. Taupin, Microemulsions and the flexibility of oil/water interfaces, J. Phys. Chem. 86 (1982), 2294-2304.
[12] J. De La Figuera, F. Leonard, N. C. Bartelt, R. Stumpf and K. F. McCarty, Nanoscale periodicity in stripe-forming systems at high temperature: \( \text{Au}/\text{W}(110) \), Phys. Rev. Lett. 100, 186102 (2008).
[13] M. Del Pino, M. Kowalczyk and J. Wei, On De Giorgi conjecture in dimension \( N \geq 9 \).
[17] J. L. Ericksen, Equilibrium of bars, J. Elasticity 5 (1975), 191-201.
[18] R. L. Fosdick and D. E. Mason, On a model of nonlocal continuum mechanics. II. Structure, asymptotics, and computations, J. Elasticity 48 (1997), 51-100.
[19] G. Fusco and J. K. Hale, Slow-motion manifolds, dormant instability, and singular perturbations, J. Dynam. Differential Equations 1 (1989), 75-94.
[20] S. Janeczko, A note on singular submanifolds, J. Geom. Phys. 2 (1985), 33-59.
[21] G. D. Kahl, Generalization of the Maxwell criterion for van der Waals equation, Phys. Rev. 155 (1967), 78.
[22] R. V. Kohn and P. Sternberg, Local minimizers and singular perturbations, Proc. Roy. Soc. Edinburgh Sect. A 111 (1989), 69-84.
[23] S. M. Muller, Singular perturbations as a selection criterion for periodic minimizing sequences, Calc. Var. Partial Differential Equations 1 (1993), 169-204.
[24] K. Nakamura, Y. Takeda, T. Akiyama and T. Ito, A. J. Freeman, Atomically sharp magnets domain wall in thin film Fe(110): a first principles noncollinear magnetism study, Phys. Rev. Lett. 93, 057202 (2004),
[25] P. D. Olmsted and S. T. Milner, Strong-segregation theory of bicontinuous phases in block copolymers, Phys. Rev. Lett. 72 (1994), 936.
[26] A. Parola and L. Reatto, Hierarchical reference theory of fluids and the critical point, Phys. Rev. A 31, (1985), 3309.
[27] G. B. Partridge, Wenhui Li, Y. A. Liao and R. G. Hulet, M. Haque and H. T. C. Stoof, Deformation of a trapped fermi gas with unequal spin populations, Phys. Rev. Lett. 97, 190407 (2006).
[28] M. Pratzer and H. J. Elmers, M. Bode, O. Pietzsch, A. Kubetzka and R. Wiesendanger, Atomic-scale magnetic domain walls in quasi-one-dimensional Fe Nanostripes, Phys. Rev. Lett., 127201 87 (2001).
[29] X. Ren and L. Truskinovsky, Fine scale microstructures in 1-D elasticity, Journal of Elasticity 59 (2000), 319-355.
[30] X. Ren and J. Wei, Wriggled lamellar solutions and their stability in the diblock copolymer problem, SIAM J. Math. Anal. 37, 455-489.
[31] P. Rosenau, Free-energy functionals at the high-gradient limit, Phys. Rev. A 41 (1990), 2227.
[32] O. Savin, Regularity of flat level sets in phase transitions, Ann. of Math. 169 (2009).
[33] S. Serfaty and I. Tice, Lorentz space estimates for the Ginzburg-Landau energy, J. Func. Anal. 254 (2008), 773-825.
[34] J. Serrin, The area rule for simple fluid phase transitions, J. Elasticity 90 (2008), 129-159.
[35] L. Truskinovsky and A. Vainchtein, Quasicontinuum models of dynamics phase transitions, Contin. Mech. Thermodyn. 18 (2006), 1-21.
[36] M. S. Turner, M. Rubinstein and C. M. Marques, Surface-induced lamellar ordering in a hexagonal phase of diblock copolymers, Macromolecules 27 (1994), 4986-4992.
[37] R. van Gastel, N. C. Bartelt, P. J. Feibelman, F. Léonard and G. L. Kellogg, Relationship between domain-boundary free energy and the temperature dependence of stress-domain patterns of Pb on Cu(111), Phys. Rev. B 70, 245413 (2004).
[38] G. M. Whitesides and M. Boncheva, Beyond molecules: Self-assembly of mesoscopic and macroscopic components, Proc. Natl. Acad. Sci, USA 99 (2002), 4769-4774.
[39] W. Windl, T. Liang, S. Lopatin and G. Duscher, Modeling and characterization of atomically sharp “perfect” Ge/SiO2 interfaces. Materials Science and Engineering B 114-115 (2004), 156-161.
[40] R. A. Young, Theory of quantum-mechanical effects on the thermodynamic properties of Lennard-Jones fluids, Phys. Rev. A 23 (1981), 1498.