Can random pinning change the melting scenario in two dimensions?

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Tuapse 17.09.2016

Motivation and Outline

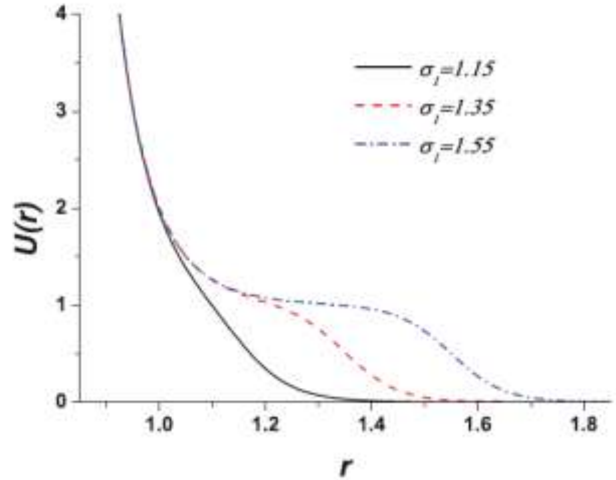
- Influence of confinement on the dynamics, thermodynamics, structural properties and anomalous behavior of core-softened systems
- Dependence of melting scenario on the shape of the core softened potential in 2D
- Influence of random pinning on the melting scenario of core-softened systems

1. Waterlike anomalies and core-softened potentials
2. Melting scenarios in 2D.
3. Phase diagram of repulsive 2D core softened system
4. Influence of random pinning on the melting scenario of 2D core-softened system

Smooth Repulsive Shoulder Potentials (Yu. D. Fomin, N.V. Gribova, V.N.Ryzhov, S.M. Stishov, and Daan Frenkel, J. Chem. Phys. **129**, 064512 (2008); Yu.D. Fomin, V.N. Ryzhov, and E.N. Tsiok, J. Chem. Phys. **134**, 044523 (2011)).

Smooth Repulsive Shoulder System (SRSS)

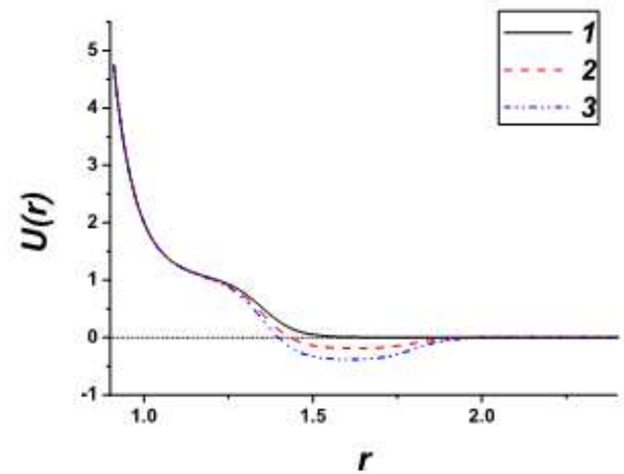
$$U(r) = \varepsilon\left(\frac{\sigma}{r}\right)^{14} + \frac{1}{2}\varepsilon(1 - \tanh(k_0[r - \sigma_1]))$$



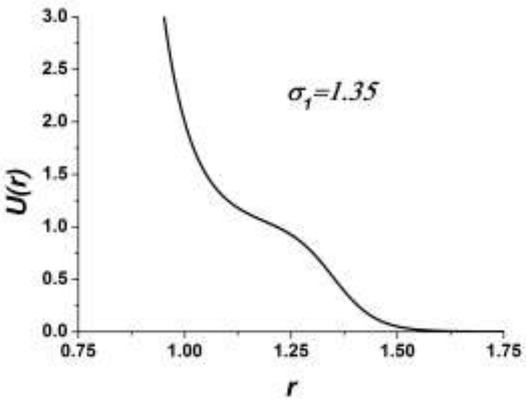
Smooth Repulsive Shoulder System With Attractive Well (SRSS-AW)

$$U(r) = \varepsilon\left(\frac{\sigma}{r}\right)^{14} + \varepsilon\,(\lambda_0 - \lambda_1 \tanh(k_1\{r - \sigma_1\}) + \lambda_2 \tanh(k_2\{r - \sigma_2\}))\,.$$

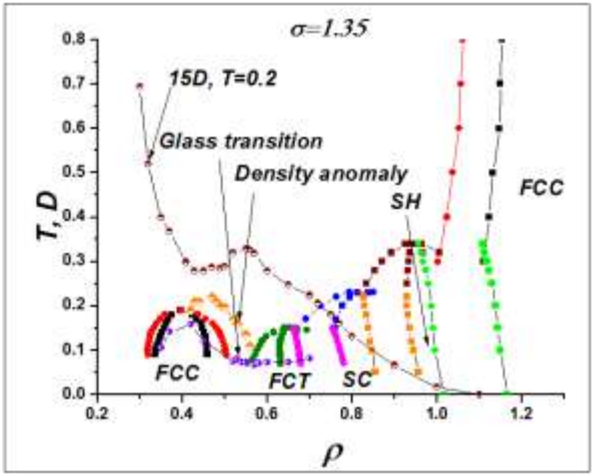
number	σ_1	σ_2	λ_0	λ_1	λ_2	well depth
1	1.35	0	0.5	0.5	0	0
2	1.35	1.80	0.5	0.60	0.10	0.20
3	1.35	1.80	0.5	0.7	0.20	0.4



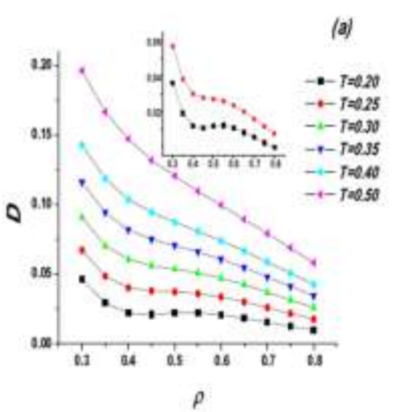
Phase diagrams and anomalies for SRSS (Yu. D. Fomin, N.V. Gribova, V.N.Ryzhov, S.M. Stishov, and Daan Frenkel, J. Chem. Phys. 129, 064512 (2008); Yu.D. Fomin, V.N. Ryzhov, and E.N. Tsiok, J. Chem. Phys. 134, 044523 (2011); Phys. Rev. E 87, 042122 (2013); R.E. Ryltsev, N.M. Chtchelkatchev, and V.N. Ryzhov, Phys. Rev. Lett. 110, 025701 (2013)).

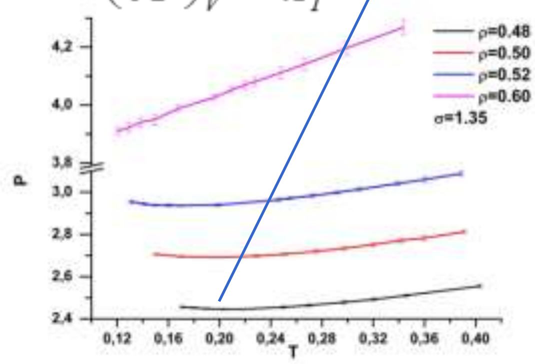


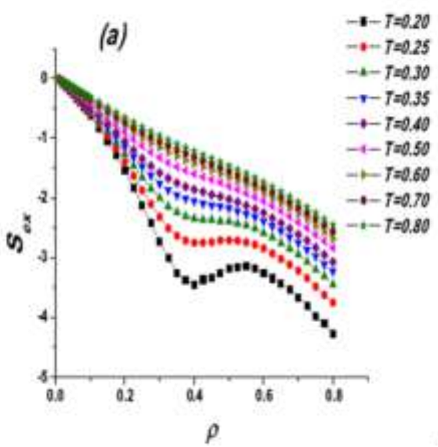
Phase diagram for σ =1.35 (with diffusion and density anomalies and glass transition).



$$\left(\frac{\partial P}{\partial T}\right)_V = \frac{\alpha_P}{\kappa_T} \qquad \kappa_T > 0 \quad \alpha_P < 0$$

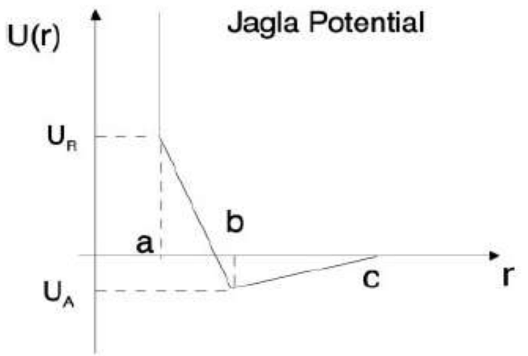






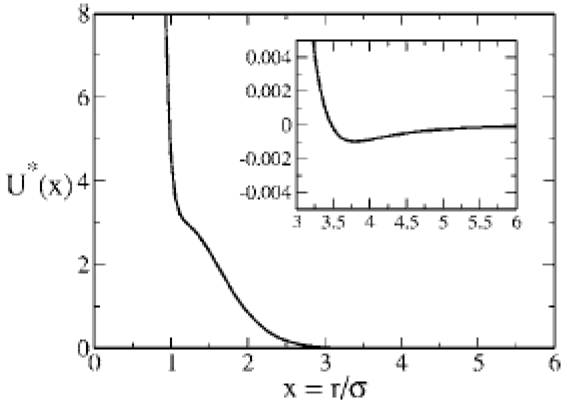
Spherically symmetric two-scale potentials

E. A. Jagla, J. Chem. Phys. 111, 8980 (1999); E. A. Jagla, Phys. Rev. E 63, 061501 (2001).



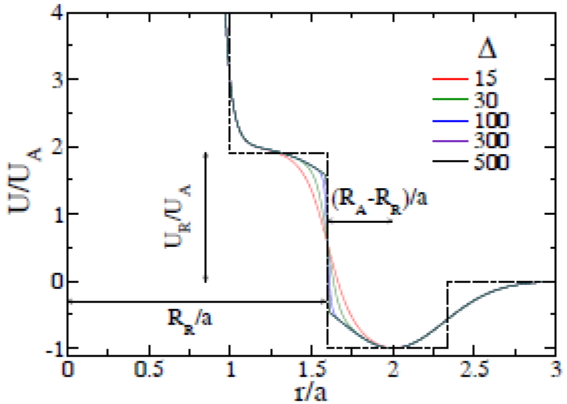
A. B. de Oliveira, P. A. Netz, T. Colla, and M. C. Barbosa, J. Chem. Phys. **124,** 084505 **(**2006).

$$U(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] + a\epsilon \exp\left[-\frac{1}{c^2}\left(\frac{r-r_0}{\sigma}\right)^2\right]$$



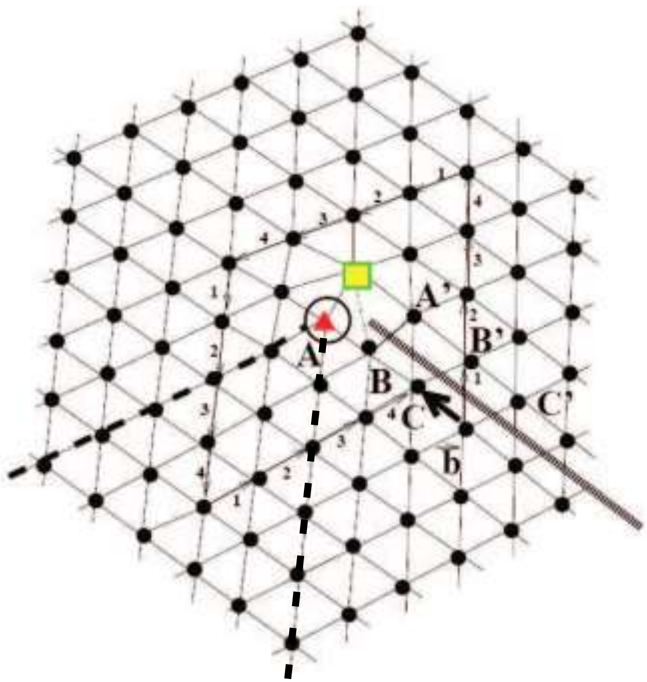
G. Franzese, J. Mol. Liq. 136, 267 2007; Pol Vilaseca and Giancarlo Franzese, J. Chem. Phys., 133, 084507 (2010).

$$U(r) = \frac{U_R}{1+\exp\left(\Delta(r-R_R)/a\right)} - U_A \exp\left[-\frac{(r-R_A)^2}{2\delta_A^2}\right] + \left(\frac{a}{r}\right)^{24}$$

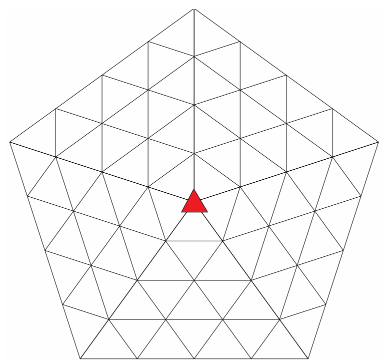


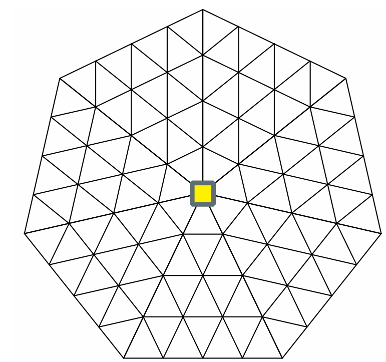
Теория двумерного плавления Березинского-Костерлица-Таулеса-Хальперина-Нельсона-Янга (BKTHNY)

Дислокации и дисклинации – базовые топологические дефекты в теории BKTHNY



Дислокация может рассматриваться как дисклинационный диполь!





Теория двумерного плавления Березинского-Костерлица-Таулеса-Хальперина-Нельсона-Янга (BKTHNY)

Упругий гамильтониан для двумерной треугольной решетки

$$H_E = \frac{1}{2}\int d^2r\ \left[2\mu u_{ij}^2 + \lambda u_{kk}^2\right],$$

где

$$u_{ij} = \frac{1}{2}\left[\frac{\partial u_i(\mathbf{r})}{\partial r_j} + \frac{\partial u_j(\mathbf{r})}{\partial r_i}\right]$$

и μ и λ - коэффициенты Ламэ.

Дислокация

$$\oint d\mathbf{u} = a_0\mathbf{b}(\mathbf{r}) = -n(\mathbf{r})a_0\mathbf{e}_1 - m(\mathbf{r})a_0\mathbf{e}_2$$

Дисклинация

$$\oint d\vartheta(\mathbf{r}) = -(2\pi/6)s, \quad s = \pm 1, \pm 2, \ldots$$

Теория двумерного плавления Березинского-Костерлица-Таулеса-Хальперина-Нельсона-Янга (BKTHNY)

Гамильтониан дислокаций

$$H_{dis} = -\frac{a_0^2 K}{8\pi} \sum_{i\neq j}^{M} \left\{ \mathbf{b}(\mathbf{r}_i)\mathbf{b}(\mathbf{r}_j) \ln \frac{r_{ij}}{a} - \frac{(\mathbf{b}(\mathbf{r}_i)\mathbf{r}_{ij})(\mathbf{b}(\mathbf{r}_i)\mathbf{r}_{ij})}{r_{ij}^2} \right\} +$$

$$+ E_d \sum_{i=1}^{M} \mathbf{b}^2(\mathbf{r}_i), \text{где } E_d \text{ - энергии ядра дислокации,}$$

$$K = \frac{4\mu(\mu+\lambda)}{2\mu+\lambda}$$

Механизм плавления – диссоциация дислокационных пар!

В точке перехода $g_{\mathbf{G}}(r) \propto r^{-\eta_G}$ $\quad 1/4 \leq \eta_G(T_m) \leq 1/3$

Выше точки перехода $\frac{a_0^2 K}{k_B T} \simeq 16\pi/(1-c|t|^\nu)$ где $t = (T-T_m)/T_m,\ \nu = 0.3696$

$g_{\mathbf{G}}(r) \propto e^{-r/\xi_+(T)}$ $\quad \xi_+(T) \propto \exp(c/|t|^\nu)$

Теория двумерного плавления Березинского-Костерлица-Таулеса-Хальперина-Нельсона-Янга (BKTHNY)

Гексатическая фаза: квазидальний ориентационный порядок при наличии дислокации!

$$u \propto \ln L \longrightarrow \omega \propto 1/L$$

Ориентационный параметр порядка для треугольной решетки

$$\psi(\mathbf{r}) = e^{6i\vartheta(\mathbf{r})}$$

Гамильтониан

$$H_A = \frac{1}{2} K_A(T) \int d^2 r \, (\nabla \vartheta(\mathbf{r}))^2 \quad H_{disc} = -\frac{\pi K_A(T)}{36} \sum_{\mathbf{r} \neq \mathbf{r}'} s(\mathbf{r}) s(\mathbf{r}') \ln \frac{|\mathbf{r} - \mathbf{r}'|}{a} + E_{cd} \sum_{\mathbf{r}} s^2(\mathbf{r})$$

$$T_i = \frac{\pi K_A(T_i)}{72 k_B T_i} \qquad < \psi^*(\mathbf{r}) \psi(0) > \propto r^{-\eta_6(T)} \qquad \eta_6(T_i) = 1/4$$

$$\xi_6 \propto \exp(b/|T - T_i|^{1/2})$$

Нерешенная проблема – нет микроскопического определения модуля Франка

KTHNY scenario of two-dimensional melting (M. Kosterlitz and D. J. Thouless, J. Phys. C 6,1181 (1973); D. R. Nelson and B. I. Halperin, Phys. Rev. B 19, 2457 (1979); A. P. Young, Phys. Rev. B 19, 1855 (1979)).

Translational and bond-orientational order in two-dimensional crystals

Is the KTHNY scenario universal?

$$g_{\mathbf{G}}(|\mathbf{r}_1 - \mathbf{r}_2|) = < \rho(\mathbf{r}_1)\rho(\mathbf{r}_2) > - \bar{\rho}^2 \propto \frac{1}{r^{k_B T \alpha_G}} \cos \mathbf{G}\mathbf{r}$$

Long-range bond-orientational order!

Transition between a crystal and an isotropic liquid can occur by means of two continuous transitions which correspond to dissociation of bound dislocation and disclination pairs, respectively.

$$g_{\mathbf{G}}(r) \propto r^{-\eta_G} \qquad \eta_G(T_m) = 1/3$$

Dislocations unbinding leads to a phase with short-range translational order,

No! First order transition is possible too.

Unbinding of disclination pairs via a continuous phase transition leads to isotropic liquid

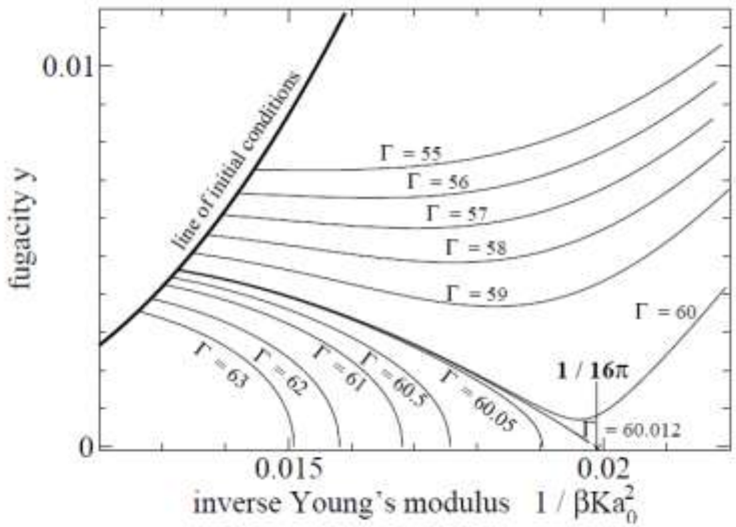
Теория двумерного плавления Березинского-Костерлица-Таулеса-Хальперина-Нельсона-Янга (BKTHNY)

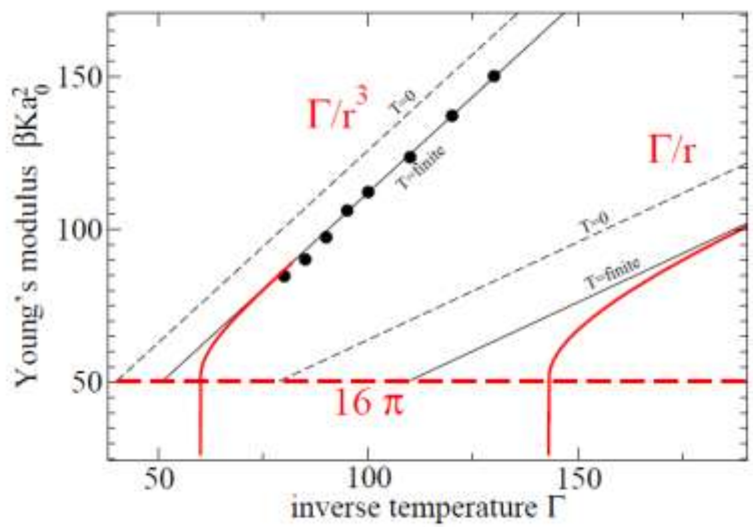
Уравнения ренормгруппы

$$\frac{dK^{-1}(l)}{dl} = \frac{3}{2}\pi y^2(l)e^{K(l)/8\pi}I_0\left(\frac{K(l)}{8\pi}\right) - \frac{3}{4}\pi y^2(l)e^{K(l)/8\pi}I_1\left(\frac{K(l)}{8\pi}\right) + O(y^3),$$

$$\frac{dy(l)}{dl} = \left[2 - \frac{K(l)}{8\pi}\right]y(l) + O(y^3).$$

$$y = e^{-E_c/k_BT}$$

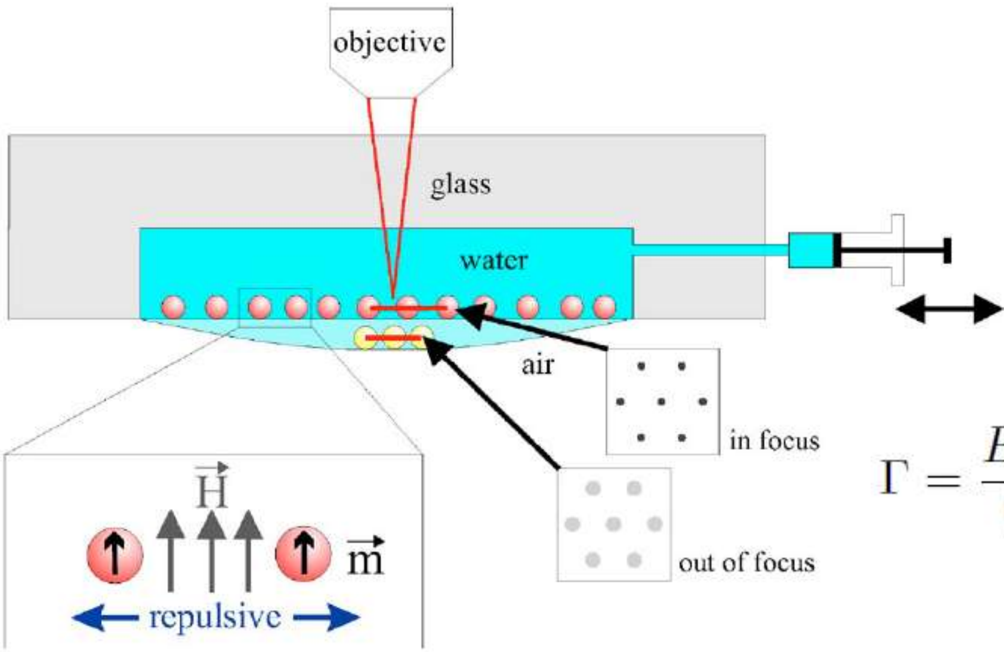




Теория двумерного плавления Березинского-Костерлица-Таулеса-Хальперина-Нельсона-Янга (BKTHNY) – экспериментальная проверка

Экспериментальная проверка – парамагнитные коллоиды

(***G.Maret et al, Phys. Rev. Lett. 82, 2721 (1999); Phys. Rev. Lett. 85, 3656 (2000); Phys. Rev. Lett. 79, 175 (1997); Phys. Rev. Lett. 92, 215504 (2004); Phys. Rev. E 75, 031402 (2007); Phys. Rev. Lett. 113, 127801 (2014); Phys. Rev. E 88, 062305 (2013); Phys. Rev. Lett. 111, 098301 (2013)***)

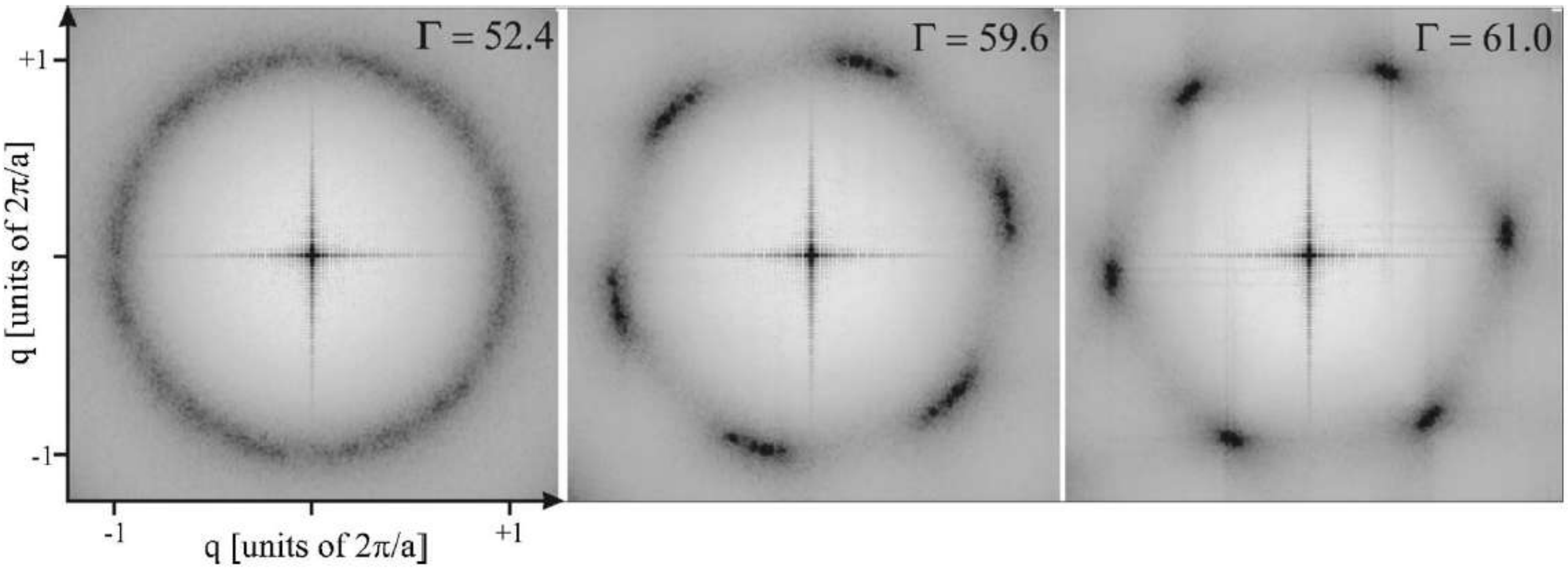


$$\beta v(r) = \frac{\Gamma}{(r/d_{nn})^3}$$

$$\Gamma = \frac{E_{magn}}{k_B T} = \frac{\mu_0}{4\pi} \cdot \frac{\chi^2 \vec{H}^2 \cdot (\pi\rho)^{3/2}}{k_B T} \propto \frac{1}{T_{sys}}$$

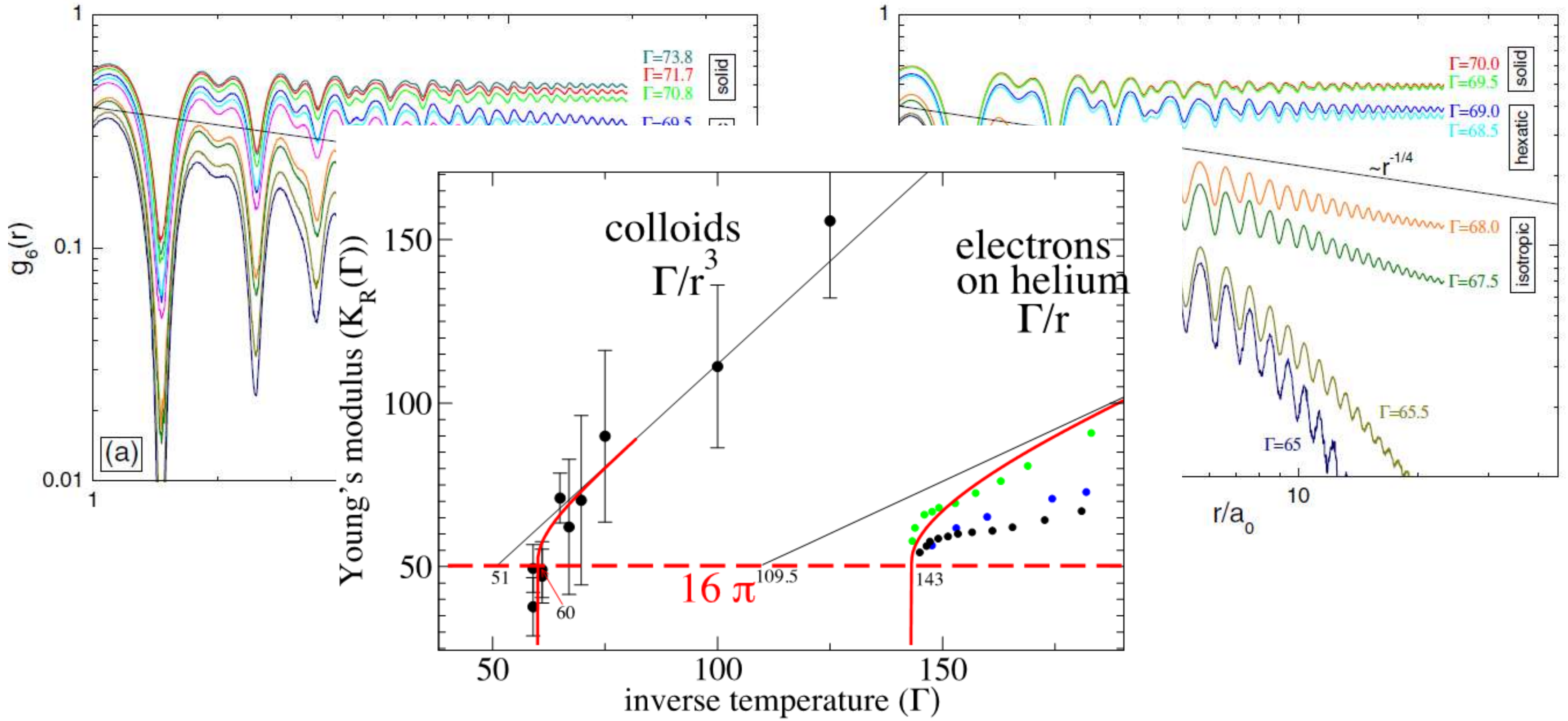
Теория двумерного плавления Березинского-Костерлица-Таулеса-Хальперина-Нельсона-Янга (BKTHNY) – экспериментальная проверка

Structure factor $S(\vec{q})$



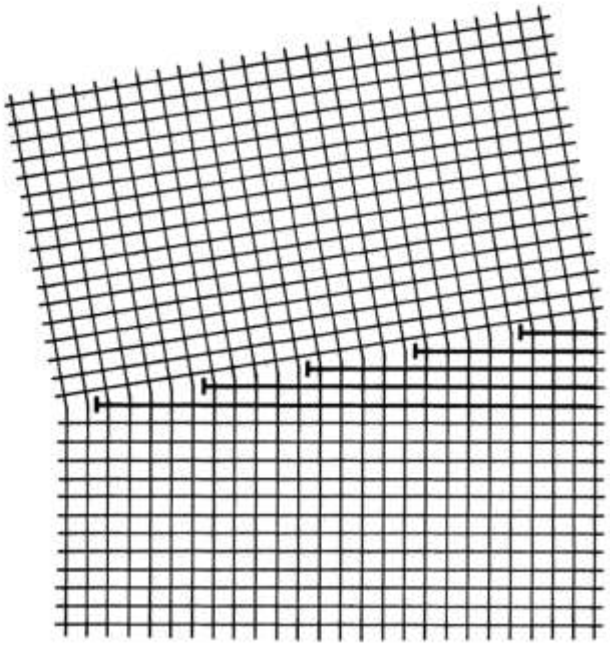
Теория двумерного плавления Березинского-Костерлица-Таулеса-Хальперина-Нельсона-Янга (BKTHNY)

Экспериментальная проверка (корреляционные функции и модуль Юнга)



Теории двумерного плавления – переход первого рода

Плавление посредством образования границ зерен
(S.T. Chui, Phys. Rev. Lett. 48, 933 (1982); Phys. Rev. B 28, 178 (1983))



$$E_c/k_BT \quad \leq \quad 2.84$$

Dissociation of disclination quadrupoles (V.N. Ryzhov, Zh. Eksp. Theor. Phys. 100, 1627 (1991)),

Melting scenarios in two-dimensions: Landau and BKTHNY theories

Order parameter $$\rho(\mathbf{r}) = \sum_{\mathbf{G}} \rho_{\mathbf{G}}(\mathbf{r}) e^{i\mathbf{G}\mathbf{r}}$$

$$F = \frac{1}{2} a_T \sum_{\mathbf{G}} |\rho_{\mathbf{G}}|^2 + b_T \sum_{\mathbf{G}_1+\mathbf{G}_2+\mathbf{G}_3=0} \rho_{\mathbf{G}_1}\rho_{\mathbf{G}_2}\rho_{\mathbf{G}_3} + O(\rho^4)$$

Landau expansion – first-order transition!

Fluctuations!

The Fourier coefficients vary slowly and have the amplitude and phase

$$\rho_{\mathbf{G}}(\mathbf{r}) = \rho_{\mathbf{G}} e^{i\mathbf{G}\mathbf{u}(\mathbf{r})}$$

*where **u(r)** has the meaning of the displacement field in the crystal. In two dimensions, the phase of the order parameter fluctuates most strongly*

Melting scenarios in two-dimensions: Landau and BKTHNY theories

The Landau expansion of the free energy with the long-wavelength fluctuations of the order parameters:

$$F = \frac{1}{2}\int \sum_{\mathbf{G}} \left[A|\mathbf{G}\times\nabla\rho_{\mathbf{G}}|^2 + B|\mathbf{G}\cdot\nabla\rho_{\mathbf{G}}|^2 + C|\rho_{\mathbf{G}}(\mathbf{G}\cdot\nabla)\rho_{\mathbf{G}}|\right] d^2r +$$

$$+\frac{1}{2}a_T\sum_{\mathbf{G}}|\rho_{\mathbf{G}}|^2 + b_T \sum_{\mathbf{G}_1+\mathbf{G}_2+\mathbf{G}_3=0} \rho_{\mathbf{G}_1}\rho_{\mathbf{G}_2}\rho_{\mathbf{G}_3} + O(\rho^4).$$

V. N. Ryzhov and E. E. Tareyeva, Phys. Rev. B 51, 8789 (1995); Physica A 314, 396-404 (2002); Physica A 432, 279–286 (2015).

The first term in expansion is the free energy of a deformed solid

$$H_E = \frac{1}{2}\int d^2r \, \left[2\mu u_{ij}^2 + \lambda u_{kk}^2\right], \qquad u_{ij} = \frac{1}{2}\left[\frac{\partial u_i(\mathbf{r})}{\partial r_j} + \frac{\partial u_j(\mathbf{r})}{\partial r_i}\right]$$

The singular part of the displacement field corresponds to dislocations and disclinations

Melting scenarios in two-dimensions: Landau and BKTHNY theories

$$F = \frac{1}{2}\int \sum_{\mathbf{G}} \left[A|\mathbf{G}\times\nabla\rho_{\mathbf{G}}|^2 + B|\mathbf{G}\cdot\nabla\rho_{\mathbf{G}}|^2 + C|\rho_{\mathbf{G}}(\mathbf{G}\cdot\nabla)\rho_{\mathbf{G}}|\right] d^2r +$$

$$+\frac{1}{2}a_T\sum_{\mathbf{G}}|\rho_{\mathbf{G}}|^2 + b_T\sum_{\mathbf{G}_1+\mathbf{G}_2+\mathbf{G}_3=0}\rho_{\mathbf{G}_1}\rho_{\mathbf{G}_2}\rho_{\mathbf{G}_3} + O(\rho^4).$$

Dislocation unbinding temperature T_m.
The modulus of the order parameter vanishes at temperature T_{MF} if the free energies of the liquid and solid phases are equal.

There are two possibilities:

1: $T_m < T_{MF}$. The system melts via two continuous transitions of the Kosterlitz–Thouless type with the unbinding of dislocation pairs.
2: $T_m > T_{MF}$. The system melts via a first-order transition because of the existence of third-order terms in the Landau expansion.

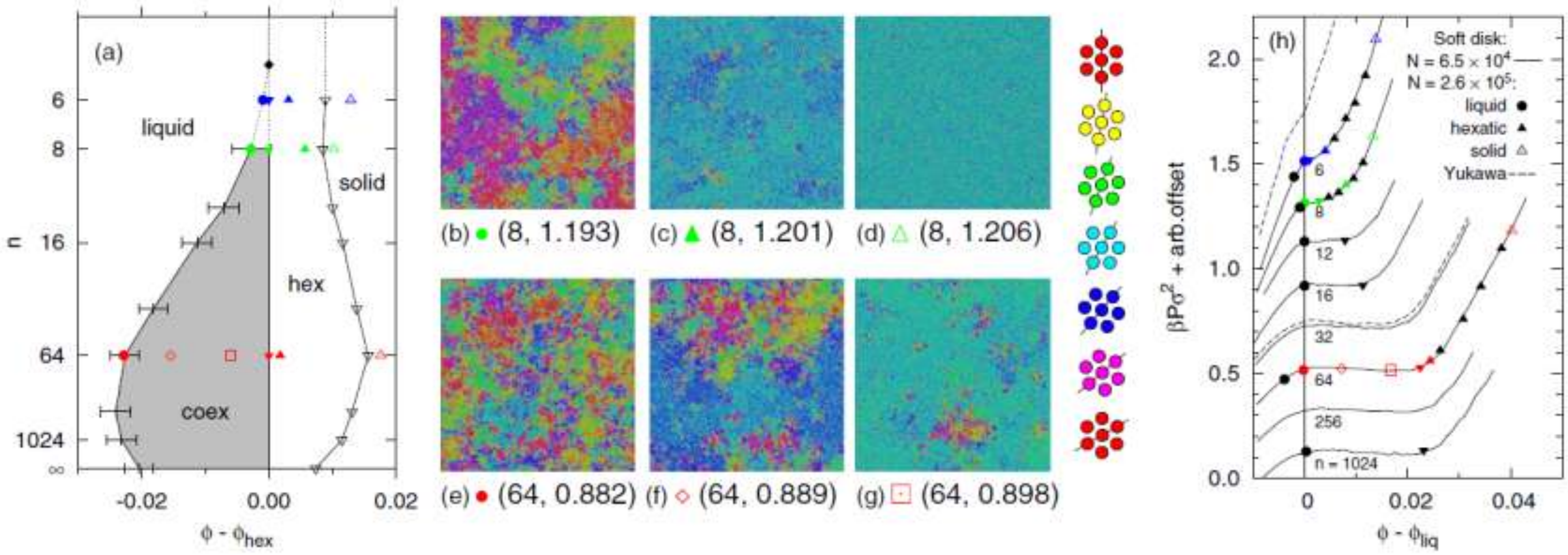
Possible scenarios: grain boundaries (S.T. Chui, Phys. Rev. Lett. 48, 933 (1982); Phys. Rev. B 28, 178 (1983)); dissociation of disclination quadrupoles (V.N. Ryzhov, Zh. Eksp. Theor. Phys. 100, 1627 (1991)), etc…

Melting scenarios in two-dimensions: First order versus continuous transition

First-order liquid-hexatic and continuous hexatic-solid transition
(E.P. Bernard and W. Krauth, Phys. Rev. Lett. 107, 155704 (2011); M.
Engel, J.A ... W. Krauth,
Phys. Rev. ... M. Dijkstra,
Soft Matte ... Rev. Lett.
114, 0357 ... Lett. 77,
2577 (199 ... X.Y. Zhao,
and Yong ... W. Qi and
M. Dijkstra, Soft Matter DOI: 10.1039/c4sm02876g).

Is it possible?

Плавление системы «мягких сфер» (S.C. Kapfer and W. Krauth, Phys. Rev. Lett. 114, 035702 (2015))

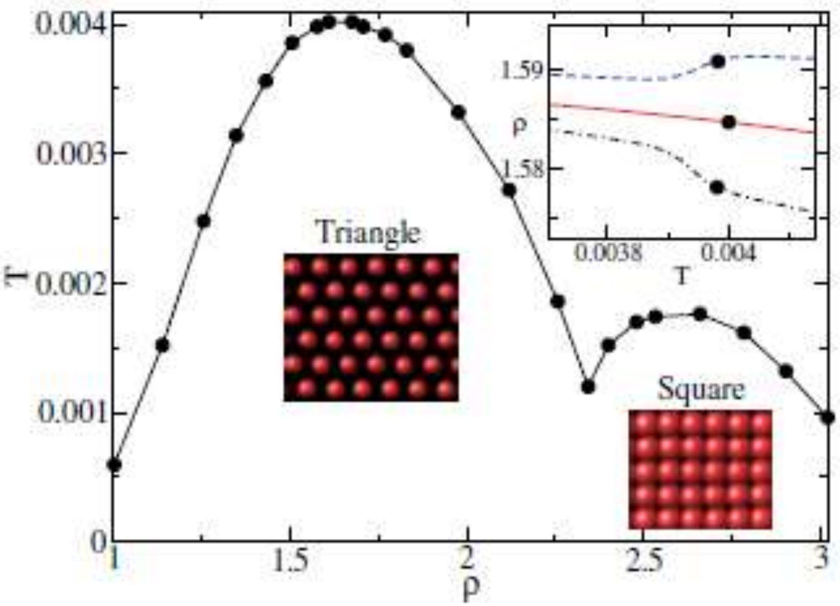


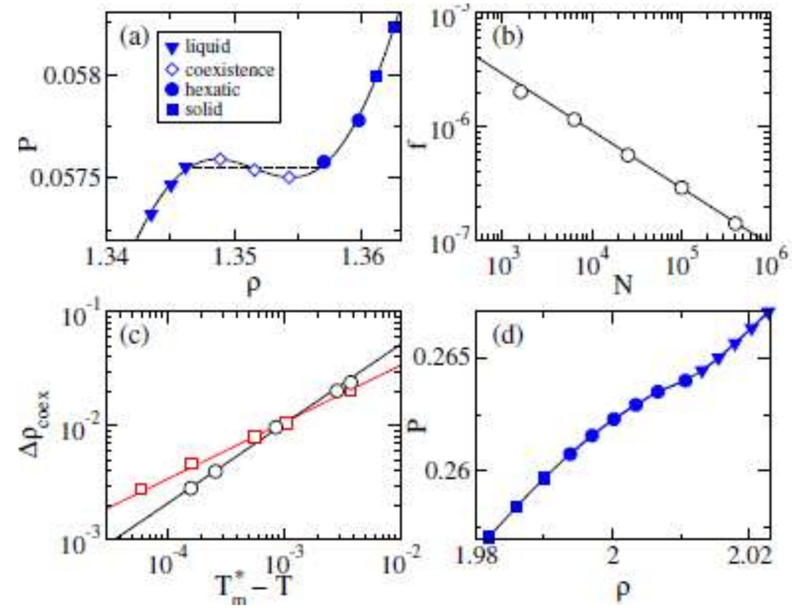
Возможный механизм – образование границ зерен ?

Density Affects the Nature of the Hexatic-Liquid Transition in Two-Dimensional Melting of Soft-Core Systems

Mengjie Zu, Jun Liu, Hua Tong, and Ning Xu*

$$U(r_{ij}) = \frac{\epsilon}{\alpha}\left(1 - \frac{r_{ij}}{\sigma}\right)^{\alpha}\Theta\left(1 - \frac{r_{ij}}{\sigma}\right),$$





nature physics

LETTERS

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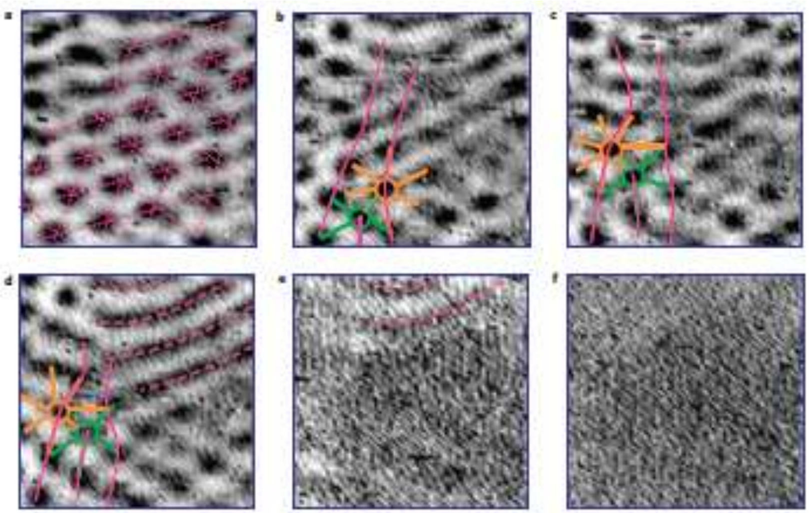
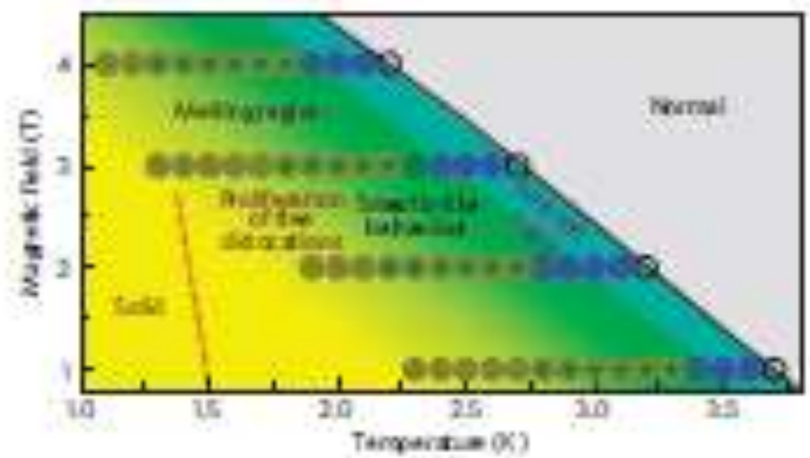
Direct observation of melting in a two-dimensional superconducting vortex lattice

I. Guillamón[1], H. Suderow[1]*, A. Fernández-Pacheco[2,3,4], J. Sesé[2,4], R. Córdoba[2,4], J. M. De Teresa[3,4], M. R. Ibarra[2,3,4] and S. Vieira[1]





Influence of random pinning on the phase diagram of core-softened system

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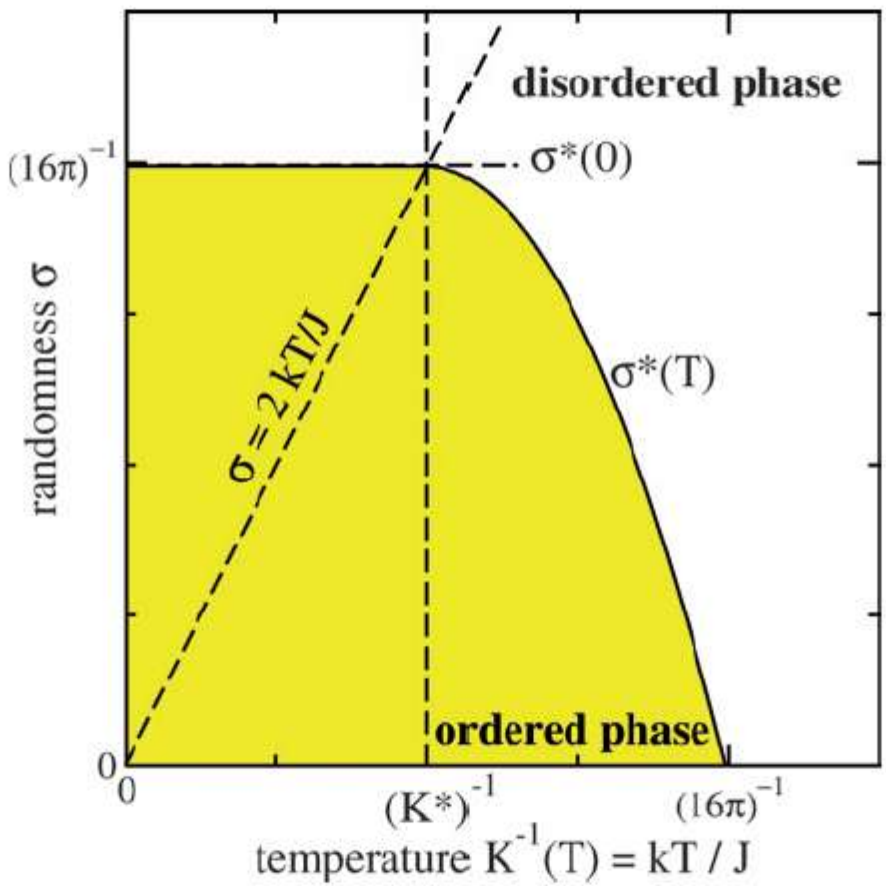
substrate *order due*
to some r

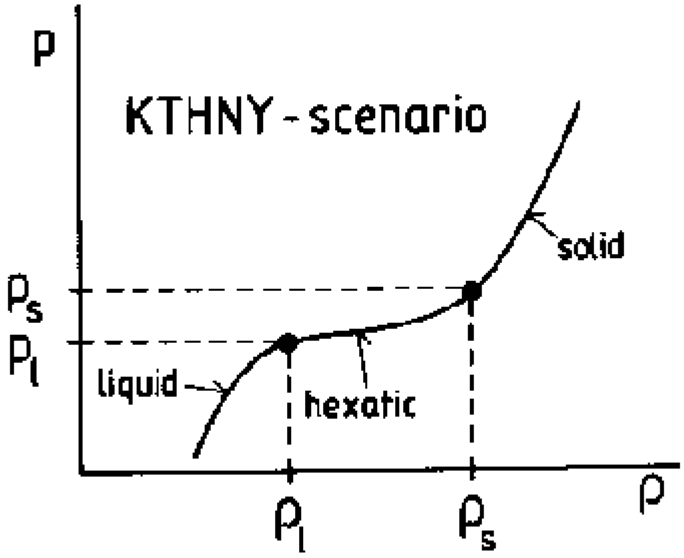


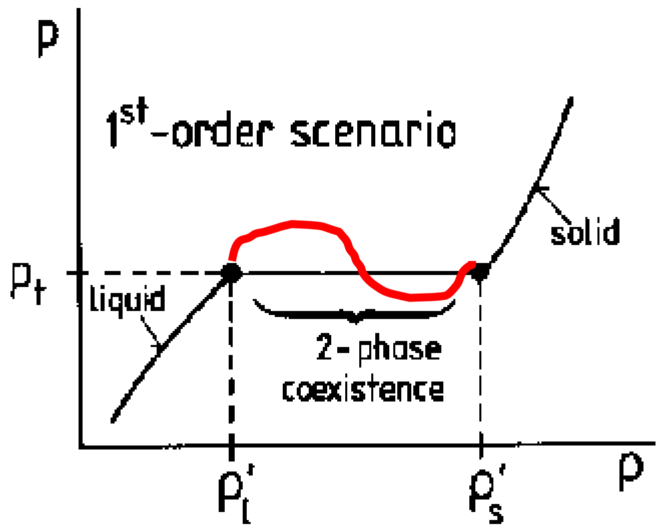
As it wa *ge melting*
scenario *R. Nelson,*
Phys. Re *n, J. Phys.*
C-Solid *and H. A.*
Fertig, P *y range of*
the hexa *hile T_i is*
predicte *eases with*
increasin *te can be*
establish

Melting scenarios in two-dimensions: First order versus continuous transition: Question: How can we distinguish the first-order and continuous transitions in simulations?

K. Binder, S. Sengupta, P. Nielaba, J. Phys.: Condens. Matter 14, 2323 (2002))

1. Isotherms

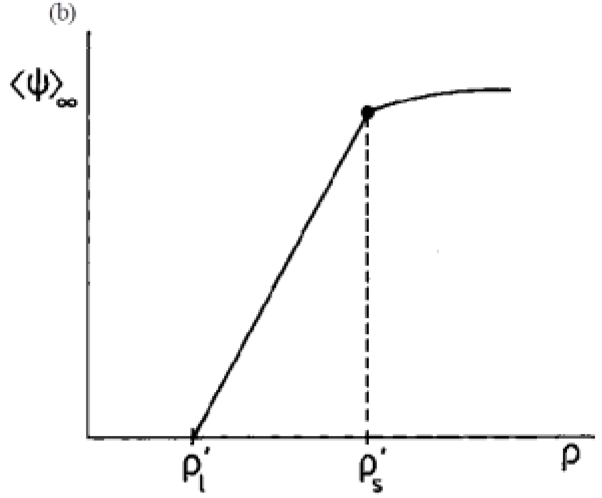




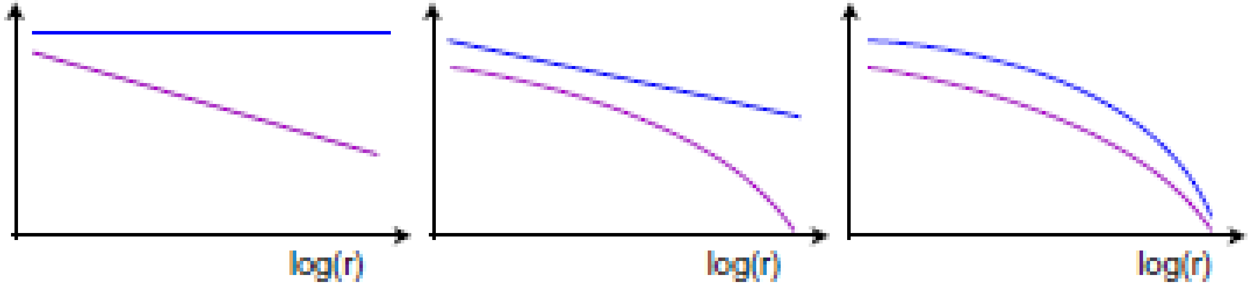
Qualitative view of the isotherms according to the BKTNY theory (left) and for the case of the first-order transition (right)

Melting scenarios in two-dimensions: First order versus continuous transition

2. A schematic diagram of the variation of the bond-orientational order parameter expected in the case of the first-order transition

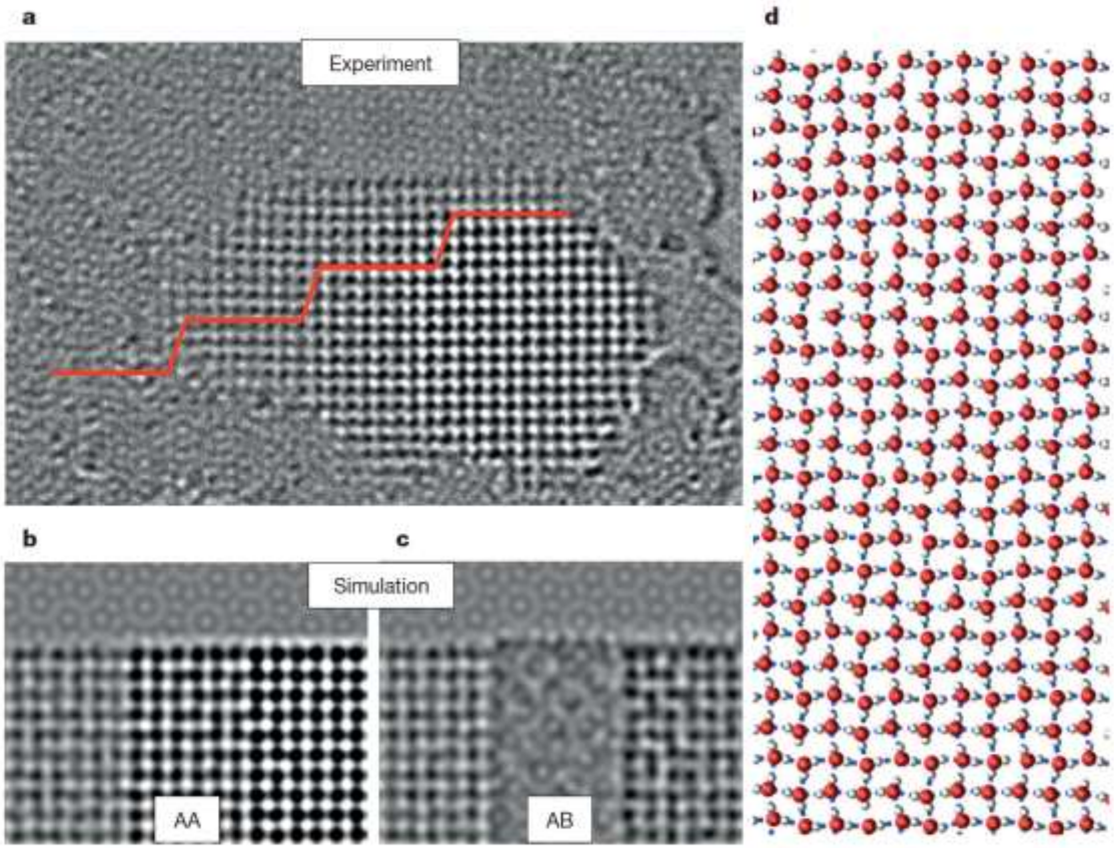


3.The schematic behaviors of the logarithms of the bond-order correlation function (blue) and the translational correlation function *(purple).*



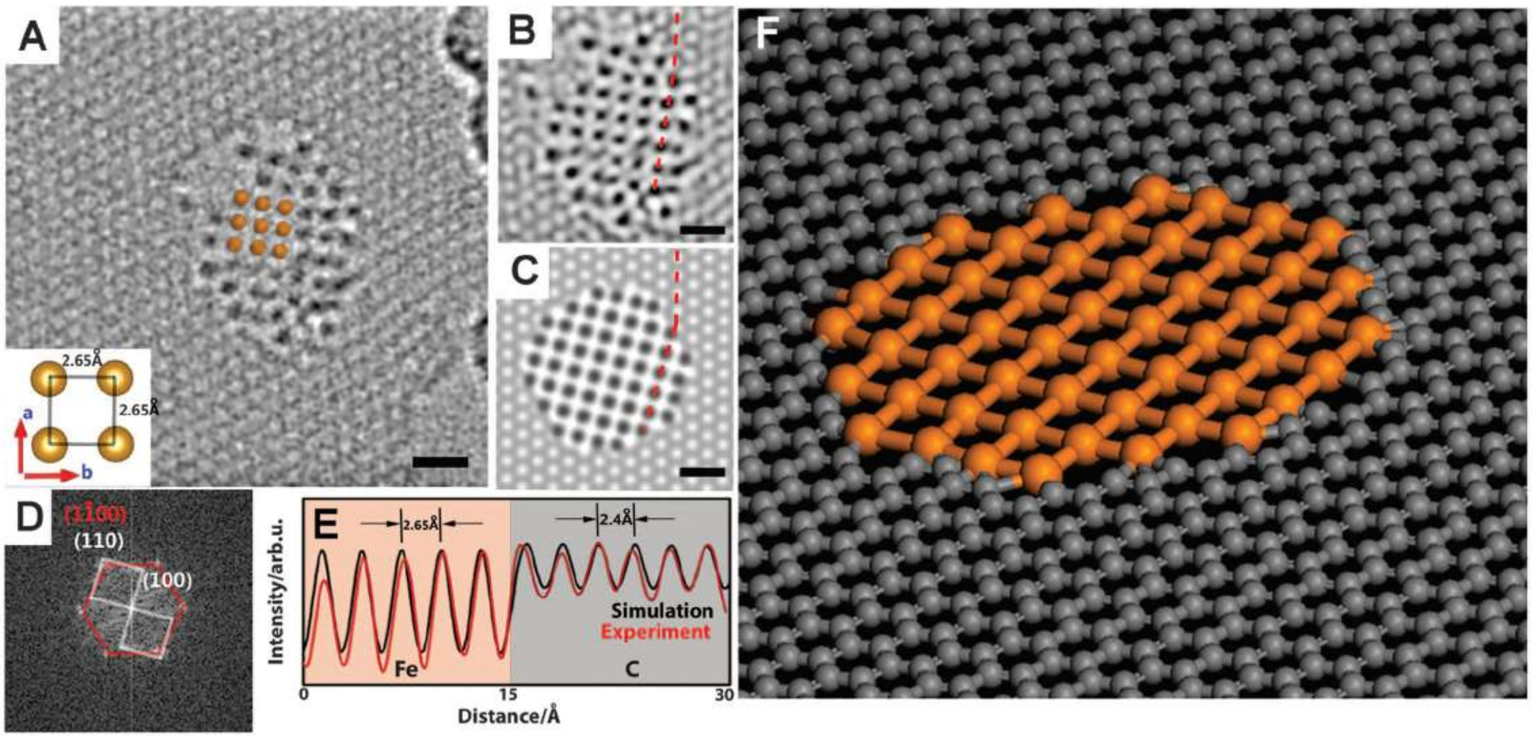
triangular crystal *hexatic phase* *isotropic liquid*

Water between two graphene sheets



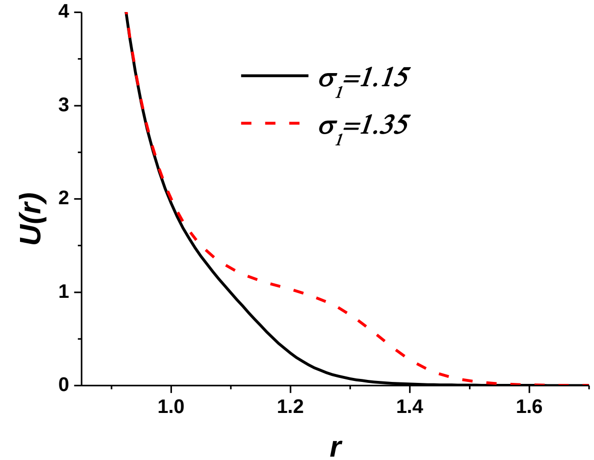
The nanoconfined between two graphene sheets water at room temperature forms 'square ice'- a phase having symmetry qualitatively different from the conventional tetrahedral geometry of hydrogen bonding between water molecules. Square ice has a high packing density with a lattice constant of 2.83A˚ and can assemble in bilayer and trilayer crystallites ***(G. Algara-Siller, O. Lehtinen, F. C. Wang, R. R. Nair, U. Kaiser, H. A.Wu, A. K. Geim & I. V. Grigorieva, NATURE 519, 443 (2015)).***

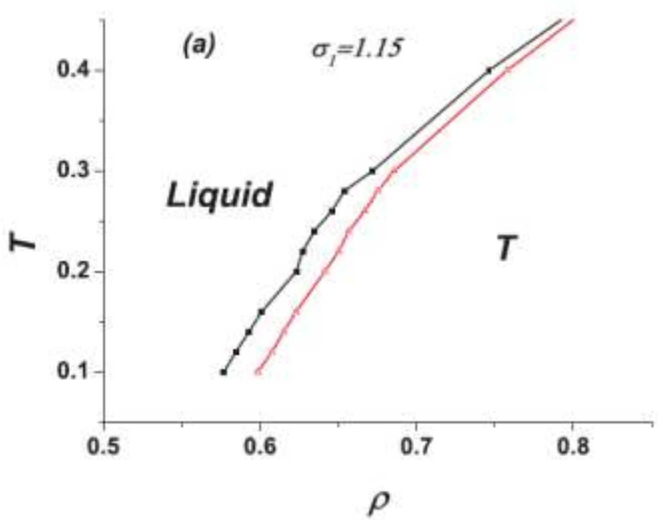
Single-Atom-Thick Iron Membranes Suspended in Graphene Pores (*Jiong Zhao et al.*, *Science* **343**, 1228 (2014))

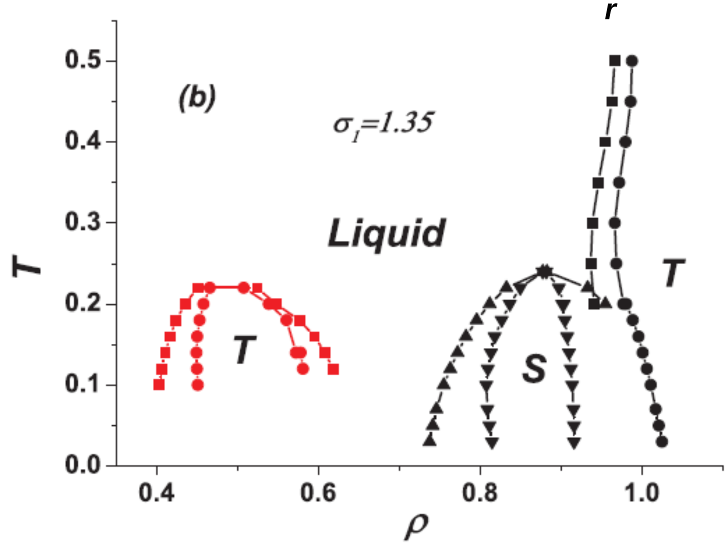


Phase diagram of the 2D core-softened system – effect of the potential softness (E. N. Tsiok, Yu. D. Fomin, and V. N. Ryzhov, Phys. Rev. E 92, 032110 (2015); arXiv: 1608.05232v1).

Helmholtz free energy calculations for different phases and a common tangent to them (D. Frenkel and B. Smit, *Understanding Molecular Simulation* (Academic, New York, 2002))







THE JOURNAL OF PHYSICAL CHEMISTRY C

Article

Formation of 2D Crystals with Square Lattice Structure from the Liquid State

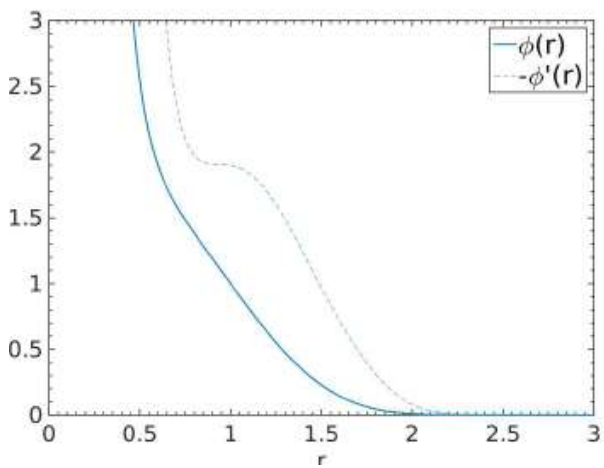
Vo Van Hoang, and Hieu Thanh Nguyen

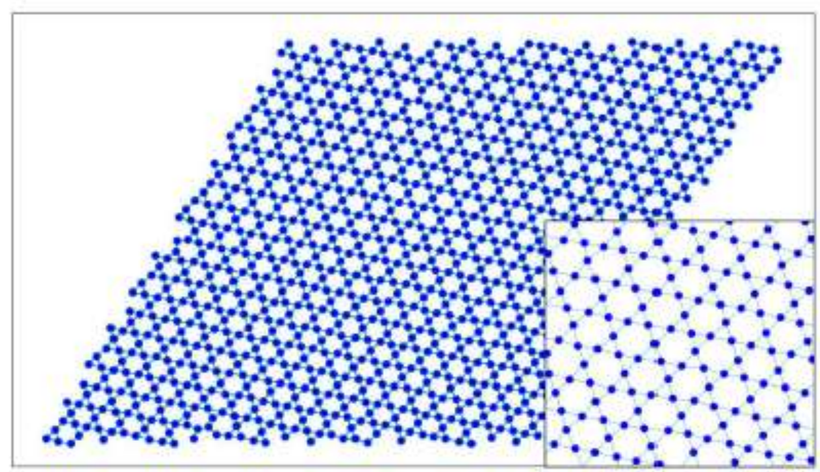
J. Phys. Chem. C, **Just Accepted Manuscript** • DOI: 10.1021/acs.jpcc.6b06704 • Publication Date (Web): 26 Jul 2016

Designing convex repulsive pair potentials that favor assembly of kagome and snub square lattices

William D. Piñeros,[1] Micheal Baldea,[2] and Thomas M. Truskett[2]
[1] *Department of Chemistry, University of Texas at Austin, Austin, TX 78712*
[2] *McKetta Department of Chemical Engineering, University of Texas at Austin, Austin, TX 78712*

(Dated: 25 July 2016)



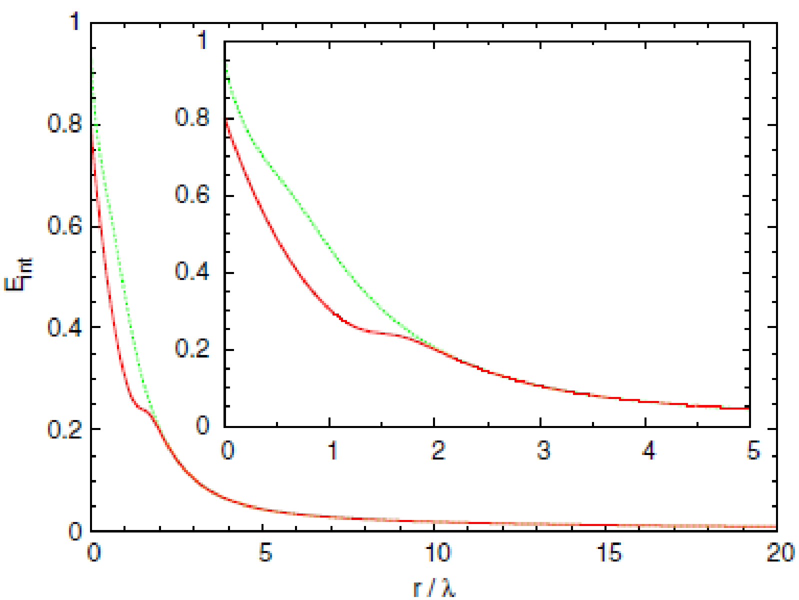


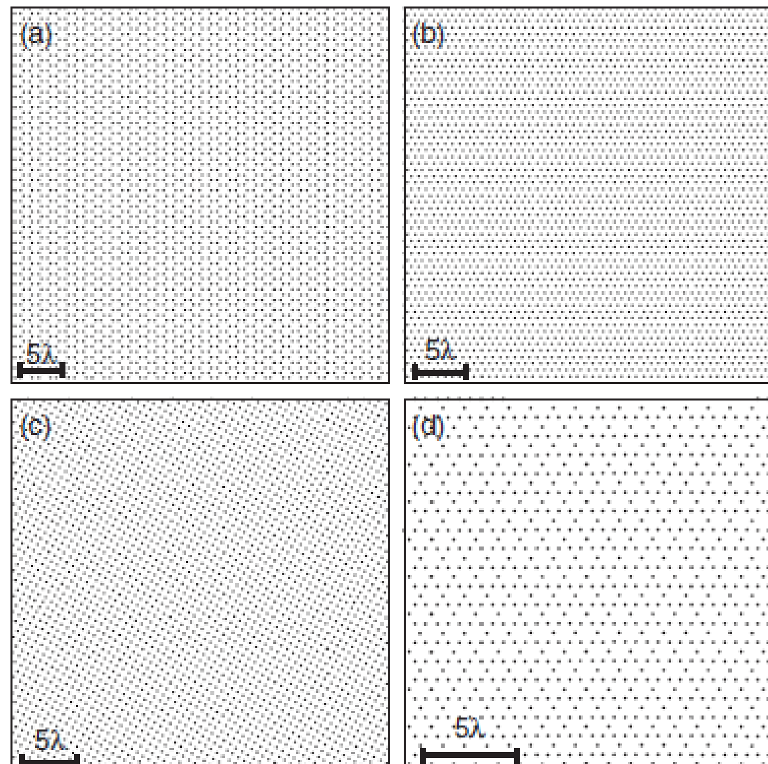
[redacted]

PHYSICAL REVIEW B **90**, 020509(R) (2014)

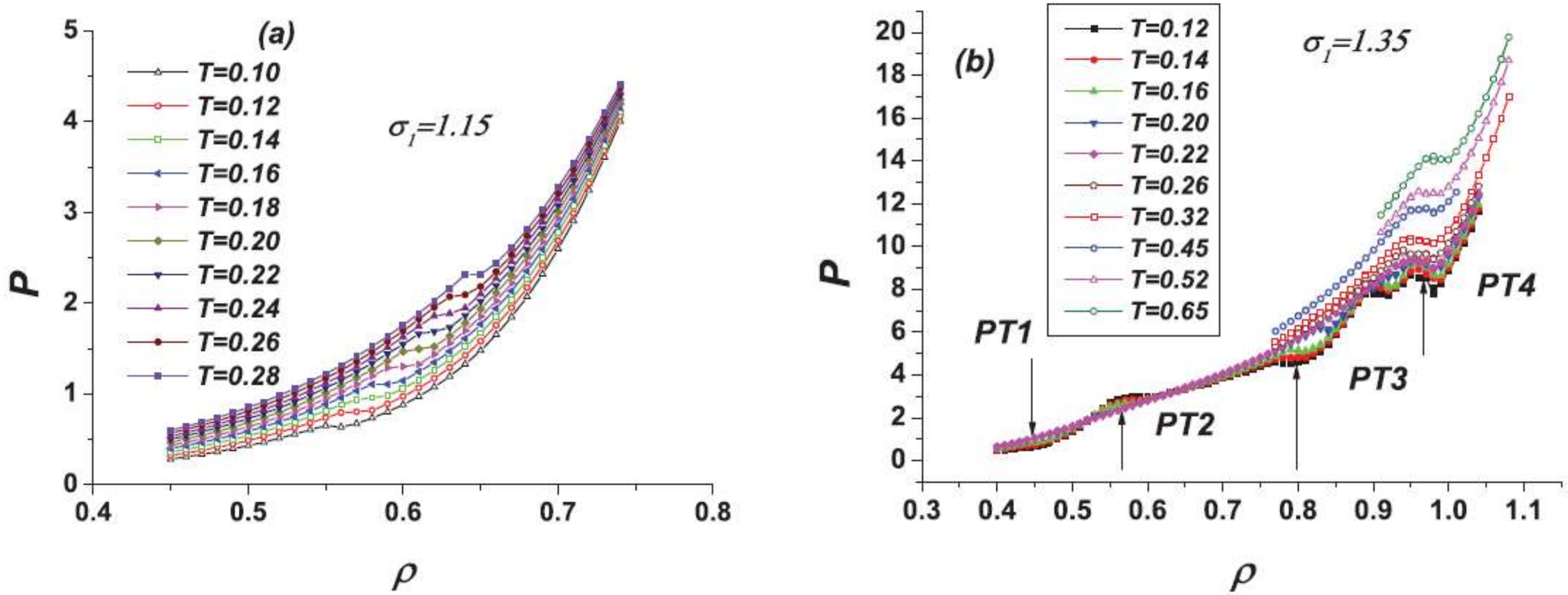
Honeycomb, square, and kagome vortex lattices in superconducting systems with multiscale intervortex interactions

Qingyou Meng,[1] Christopher N. Varney,[2] Hans Fangohr,[3] and Egor Babaev[4,1]





Melting transition in core-softened system - effect of the potential softness (D.E. Dudalov, Yu.D. Fomin, E.N. Tsiok, and V.N. Ryzhov, Phys. Rev. Lett. 112, 157803 (2014); Soft Matter 10, 4966 (2014); J. Chem. Phys. 141, 18C522 (2014); arXiv: 1608.05232v1).



For σ=1.15 one liquid-solid first order transition ???

For σ=1.35 there are several transitions, corresponding to the phase diagram at the previous slide.

However, more detailed study is necessary!

Melting transition in core-softened system

Bond orientational and translational order parameters

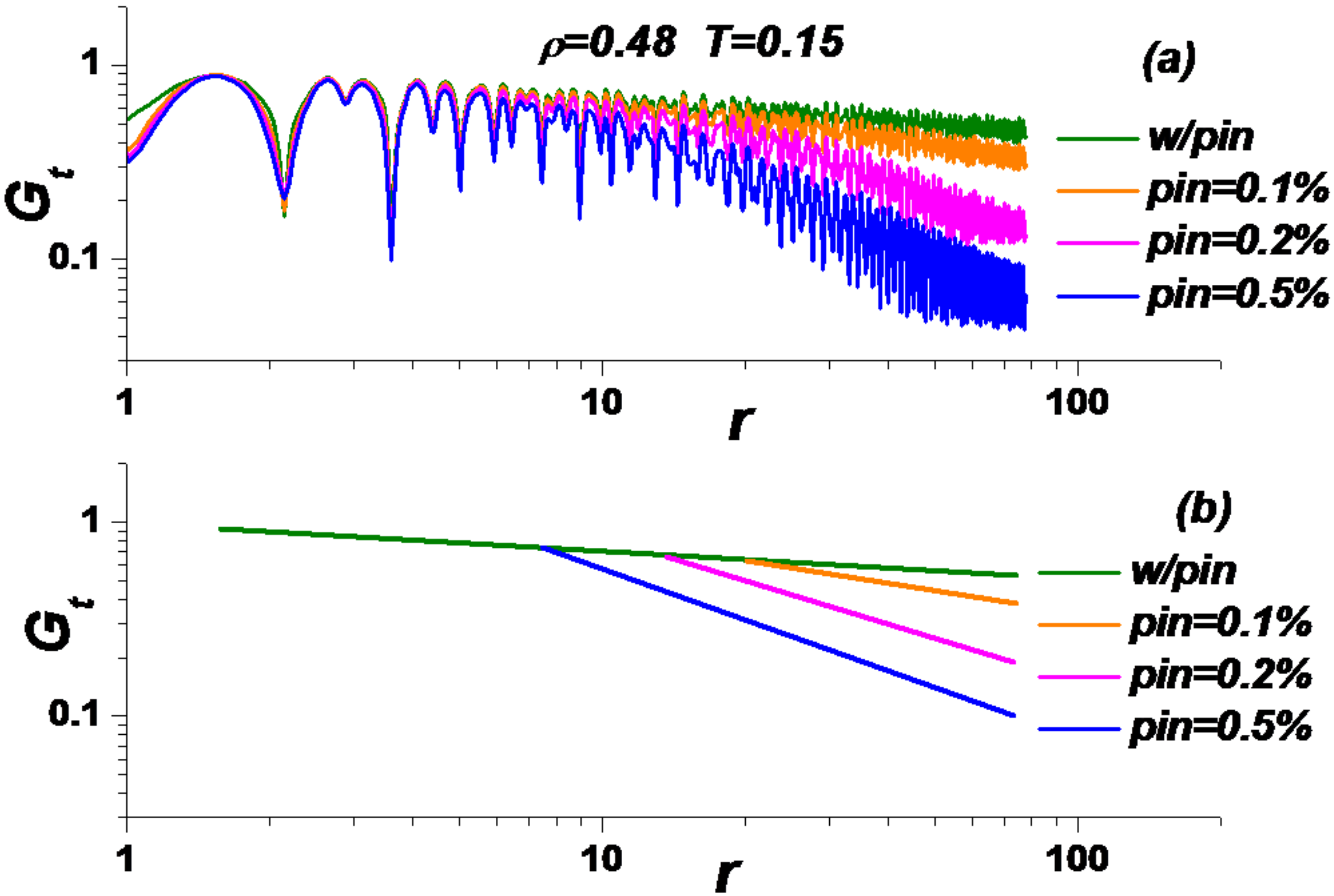
$$\Psi_6(\mathbf{r_i}) = \frac{1}{n(i)} \sum_{j=1}^{n(i)} e^{in\theta_{ij}} \quad \psi_6 = \frac{1}{N}\left\langle\left\langle\left|\sum_i \Psi_6(\mathbf{r}_i)\right|\right\rangle\right\rangle_{rp} \quad \psi_T = \frac{1}{N}\left\langle\left\langle\left|\sum_i e^{i\mathbf{G}\mathbf{r}_i}\right|\right\rangle\right\rangle_{rp}$$

The orientational correlation function $G_6(r)$

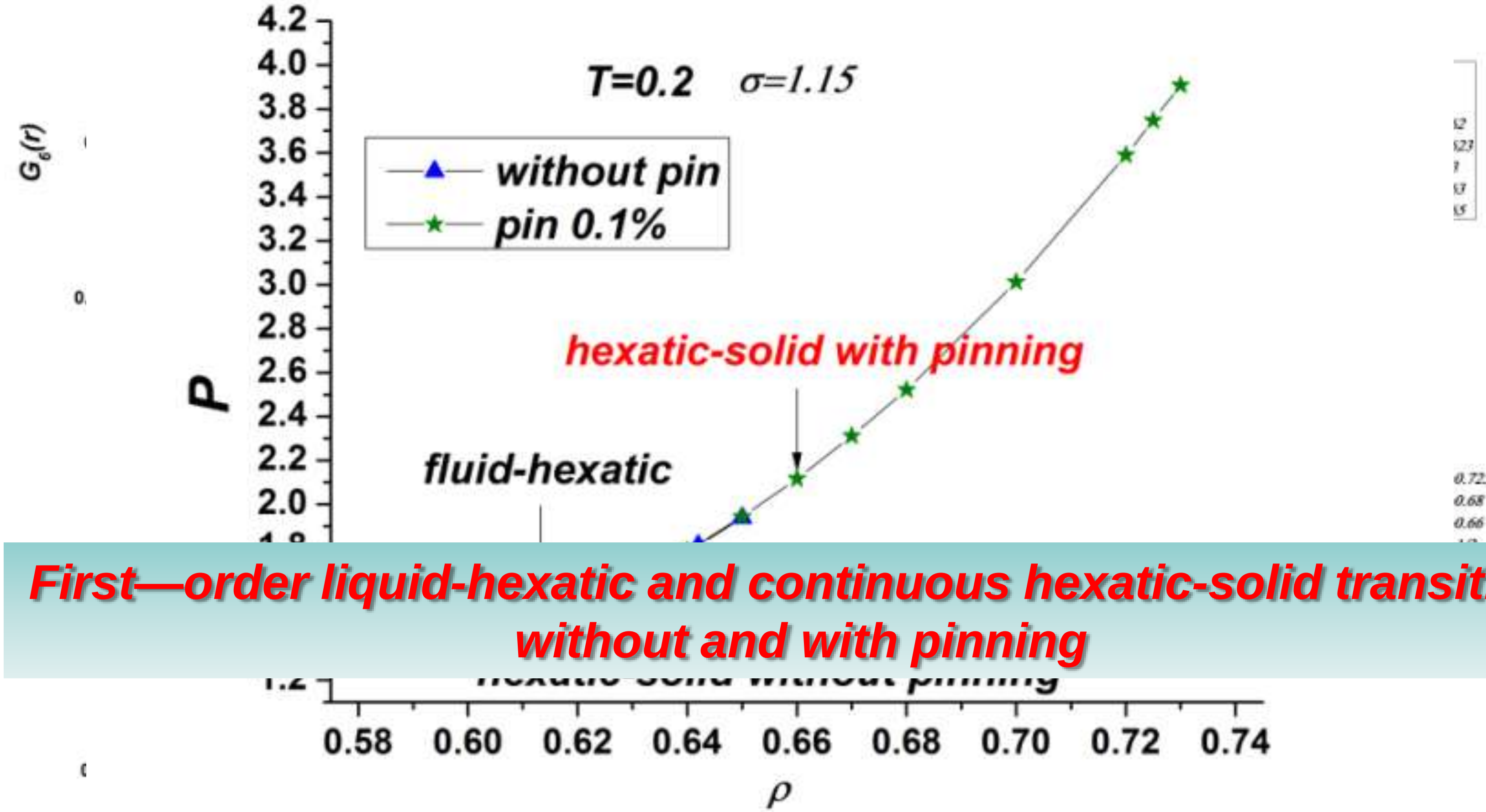
The translational correlation function $G_T(r)$

$$G_6(r) = \left\langle \frac{\langle \Psi_6(\mathbf{r})\Psi_6^*(\mathbf{0})\rangle}{g(r)} \right\rangle_{rp} \qquad G_T(r) = \left\langle \frac{< \exp(i\mathbf{G}(\mathbf{r}_i - \mathbf{r}_j)) >}{g(r)} \right\rangle_{rp}$$

Dependence of translational correlation functions on the random pinning concentrations (E. N. Tsiok, D.E. Dudalov, Yu. D. Fomin, and V. N. Ryzhov, Phys. Rev. E 92, 032110 (2015)).

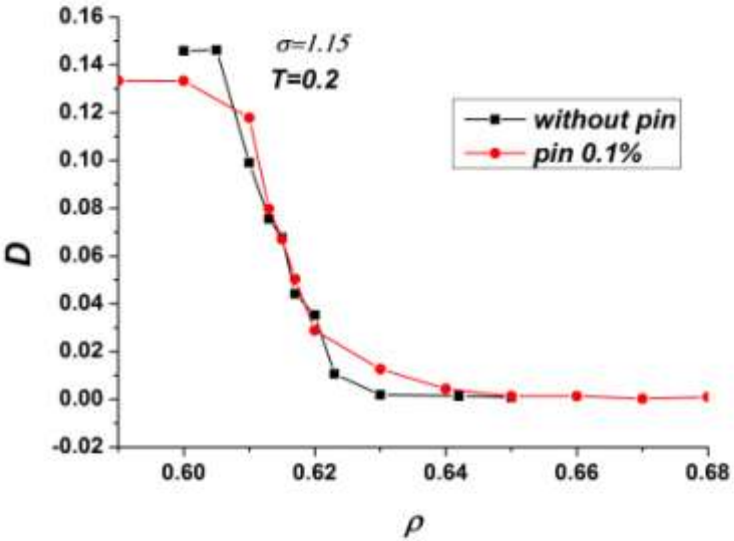


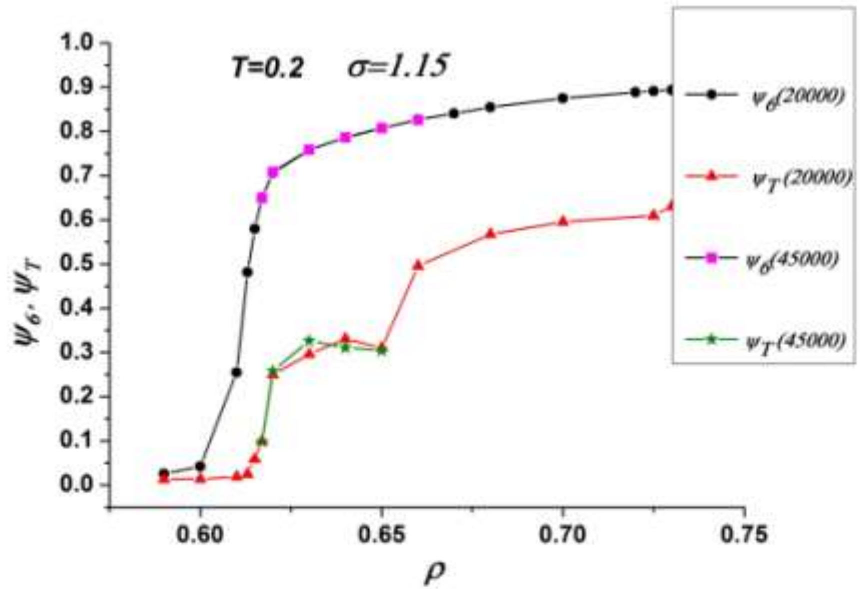
Melting transition in core-softened system for σ=1.15 without and with random pinning



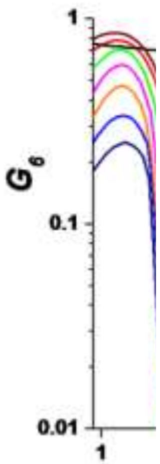
First—order liquid-hexatic and continuous hexatic-solid transitions without and with pinning

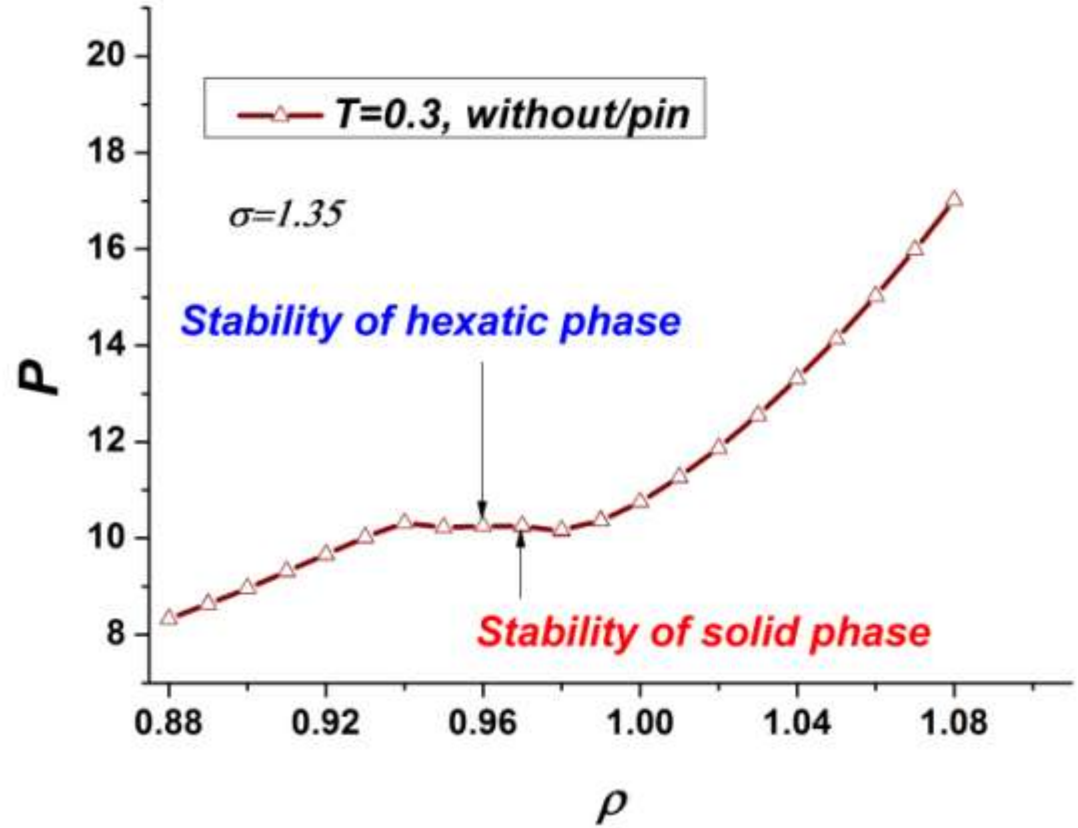
Diffusion, orientational ψ_6 and translational ψ_T order parameters for σ=1.15 with random pinning

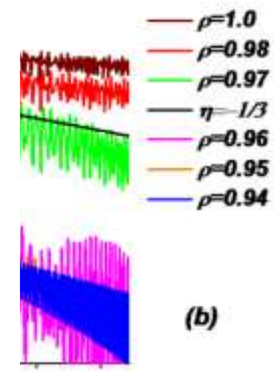




Melting transition in core-softened system with σ=1.35 at high densities without pinning

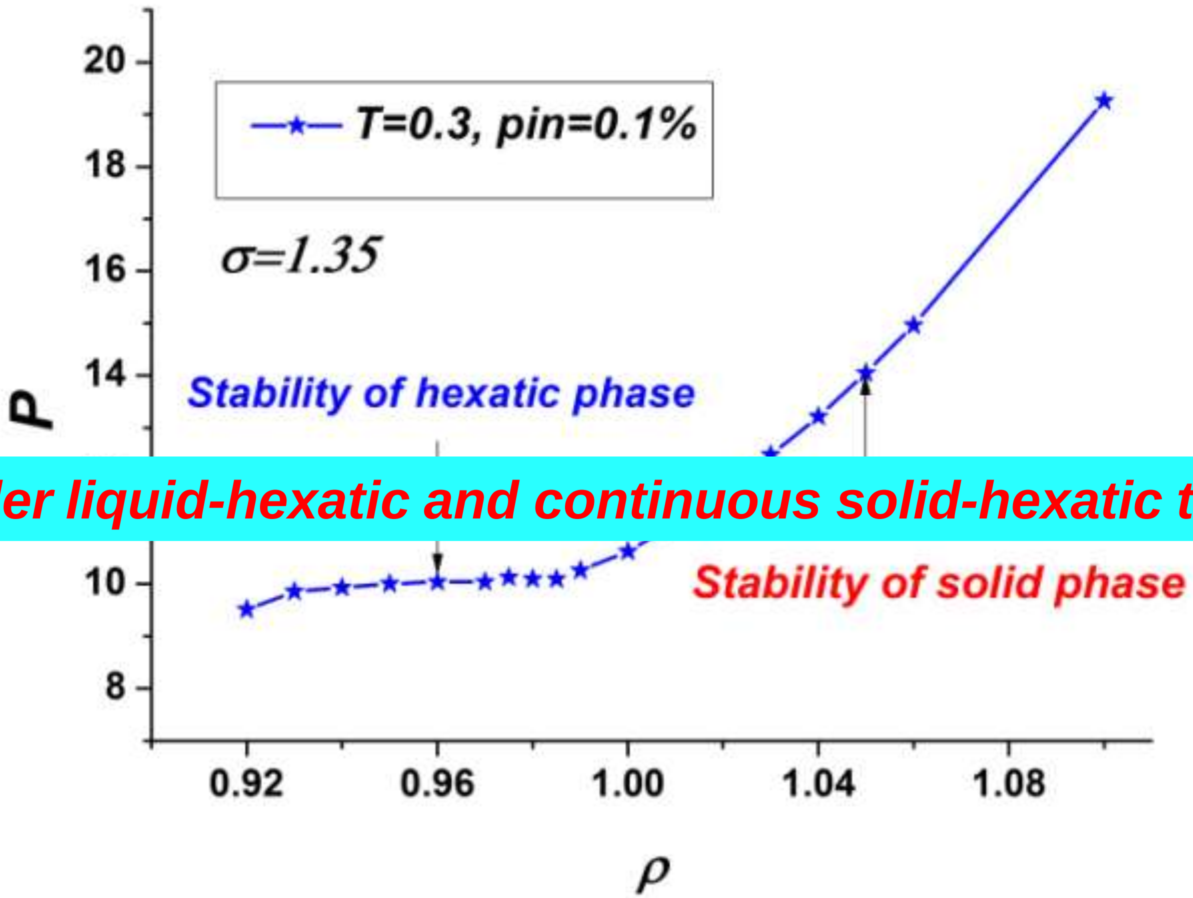






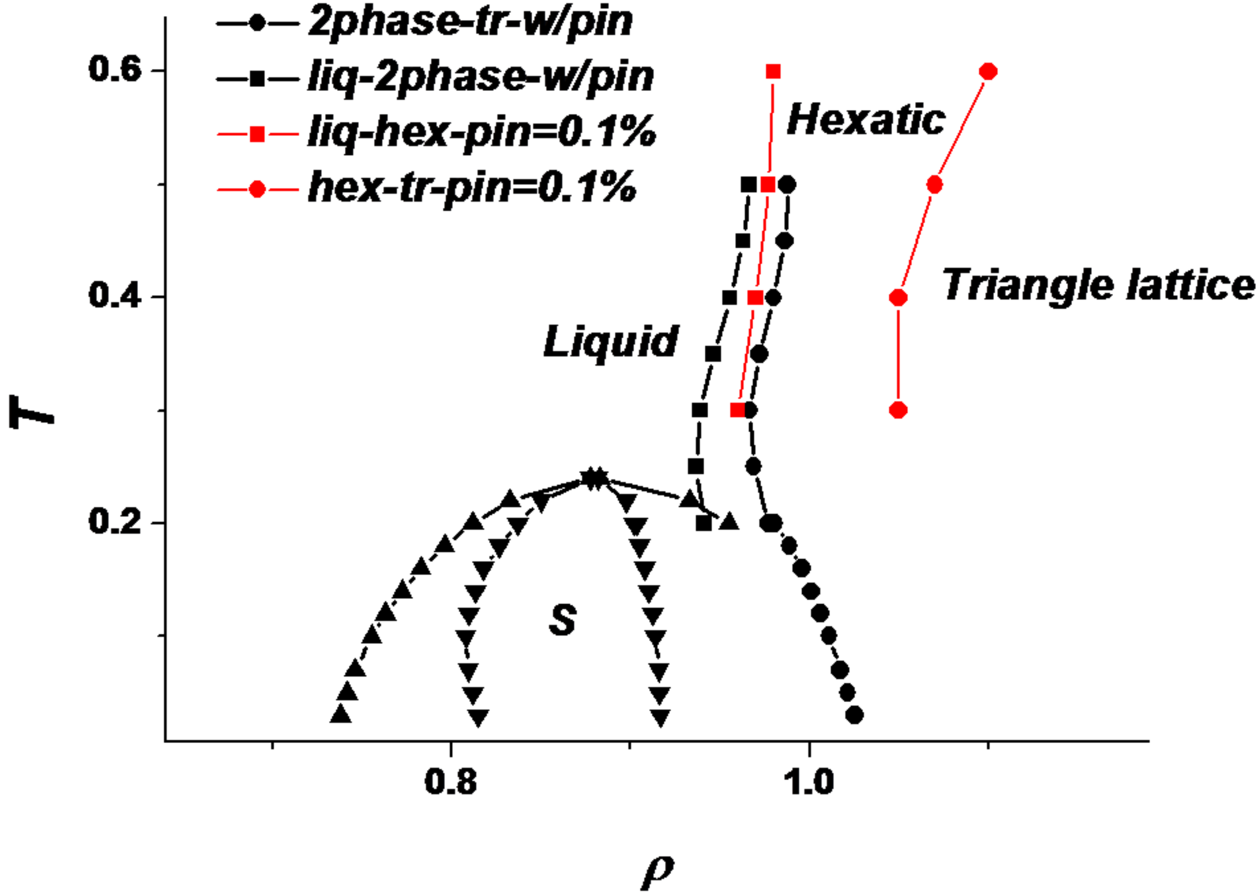
First-order transition!

Melting transition in core-softened system with σ=1.35 at high densities with random pinning

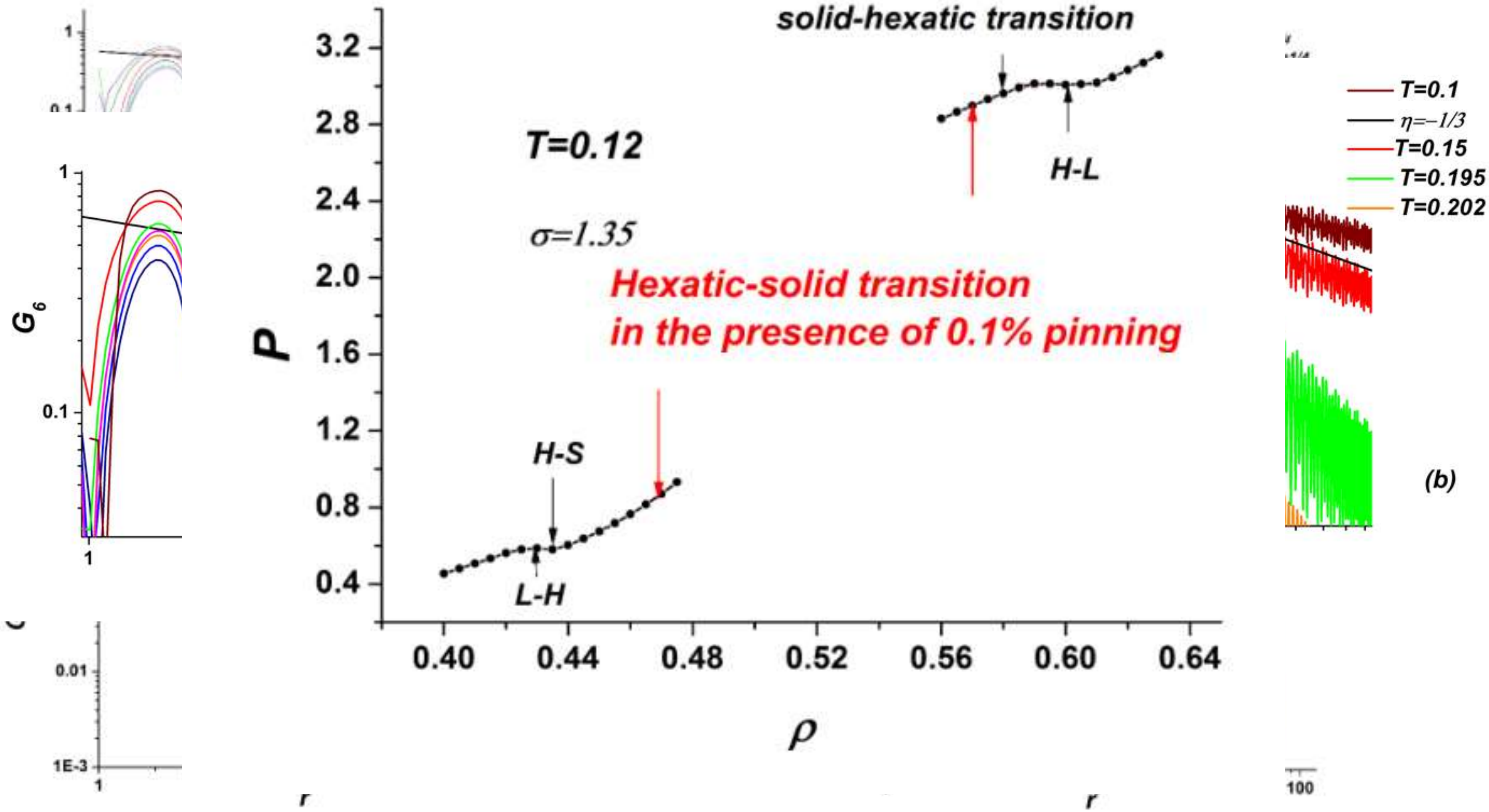


First-order liquid-hexatic and continuous solid-hexatic transitions

Phase diagram in the presence of pinning – high densities σ=1.35 (E. N. Tsiok, D.E. Dudalov, Yu. D. Fomin, and V. N. Ryzhov, Phys. Rev. E 92, 032110 (2015)).

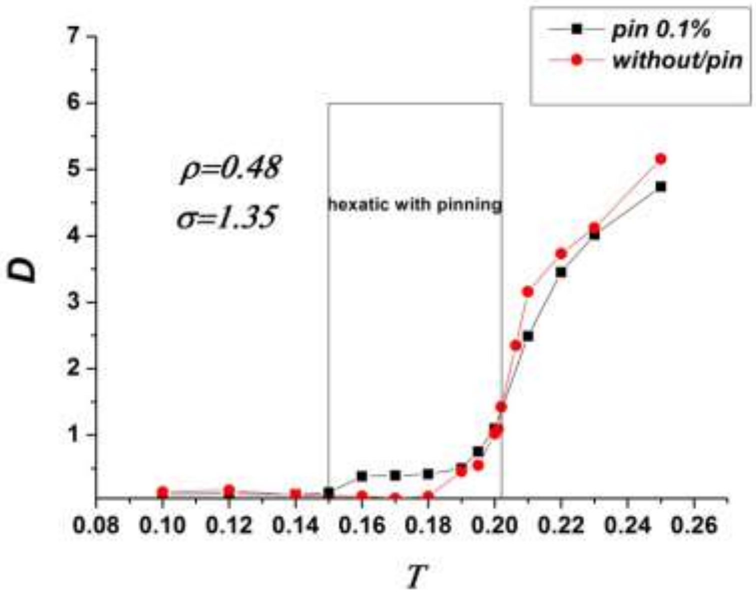


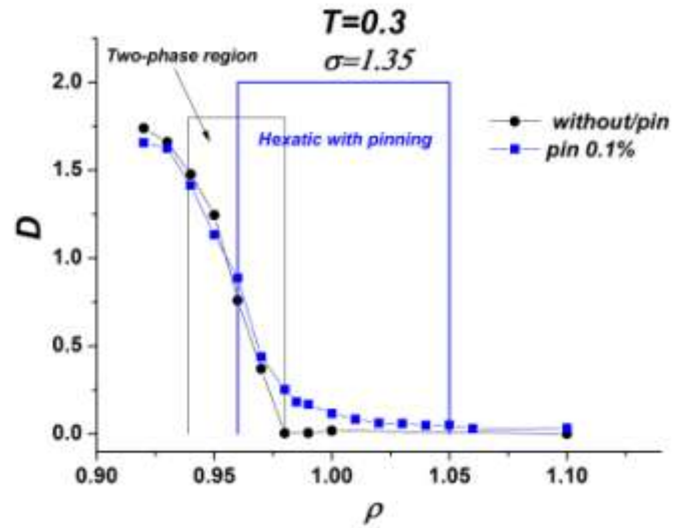
Phase diagram in the presence of pinning – low densities σ=1.35

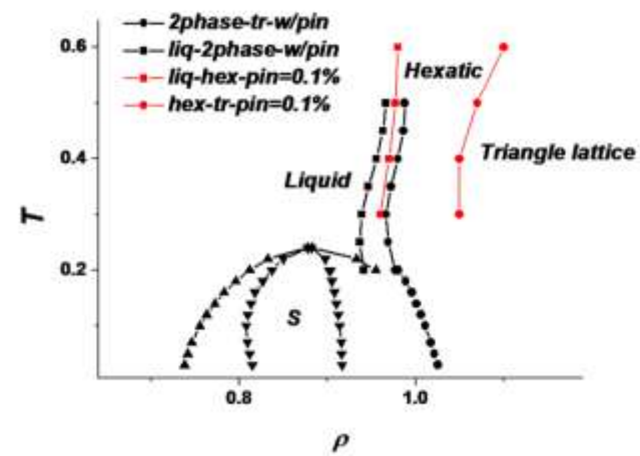


Hertzian disks: M. Zu et al, arXiv:1605.00747

Diffusion in the presence of random pinning σ=1.35







Conclusions

1). In the talk we present a molecular dynamics study of the two dimensional core-softened system without and in the presence of the random pinning. It is shown that the melting scenario drastically depends on the form of the potential. In our system melting can occur through a first-order phase transition and as a result of two transitions with the intermediate hexatic phase - first-order liquid-hexatic and continuous hexatic-solid transition.

2). The influence of the random pinning on the phase diagram is investigated. It is shown that pinning transforms the first order melting in two transitions: first-order liquid-hexatic transition and continuous hexatic-solid transition. In the case the two-stage melting pinning drastically widens the hexatic phase.

3). There is no adequate theory of a first-order liquid-hexatic transition.

Thank you very much for your attention

Melting scenarios in two-dimensions: Landau and BKTHNY theories of liquid-hexatic transition

Order parameter $F_2(\mathbf{r}) = g(r)(1 + f(\mathbf{r}_0))$ $f(\mathbf{r}_0) = \sum_m f_m e^{im\theta}$

Mean-field expansion – transition at T_{MF} $\Delta F = a_6(T - T_c) f_6^2 + b f_6^4$

Fluctuations of the order parameter phase in 2D

$$f_m(\mathbf{r}) = f_m^0 e^{i\phi(\mathbf{r})}$$

BKT liquid-hexatic transition

$$\Delta F = \int \left(\frac{1}{2} K_A (f_6^0)^2 (\nabla\phi)^2 + a_6(T - T_c)(f_6^0)^2 + b(f_6^0)^4 \right) d\mathbf{r}$$

Unbinding of the singular topological defects of the order-parameter phase (disclinations) at T_i - BKT transition. Continuous transition at T_i and at T_{MF}.

What is the mechanism of the first-order liquid-hexatic transition (grain-boundaries like mechanism)?

Melting scenarios in two-dimensions: Landau and BKTHNY theories

Order parameter $$\rho(\mathbf{r}) = \sum_{\mathbf{G}} \rho_{\mathbf{G}}(\mathbf{r}) e^{i\mathbf{G}\mathbf{r}}$$

$$F = \frac{1}{2} a_T \sum_{\mathbf{G}} |\rho_{\mathbf{G}}|^2 + b_T \sum_{\mathbf{G}_1+\mathbf{G}_2+\mathbf{G}_3=0} \rho_{\mathbf{G}_1}\rho_{\mathbf{G}_2}\rho_{\mathbf{G}_3} + O(\rho^4)$$

Landau expansion – first-order transition!

Fluctuations!

The Fourier coefficients vary slowly and have the amplitude and phase

$$\rho_{\mathbf{G}}(\mathbf{r}) = \rho_{\mathbf{G}} e^{i\mathbf{G}\mathbf{u}(\mathbf{r})}$$

*where **u(r)** has the meaning of the displacement field in the crystal. In two dimensions, the phase of the order parameter fluctuates most strongly*

Melting scenarios in two-dimensions: Landau and BKTHNY theories

The Landau expansion of the free energy with the long-wavelength fluctuations of the order parameters:

$$F = \frac{1}{2}\int \sum_{\mathbf{G}} \left[A|\mathbf{G}\times\nabla\rho_{\mathbf{G}}|^2 + B|\mathbf{G}\cdot\nabla\rho_{\mathbf{G}}|^2 + C|\rho_{\mathbf{G}}(\mathbf{G}\cdot\nabla)\rho_{\mathbf{G}}|\right] d^2r +$$

$$+\frac{1}{2}a_T\sum_{\mathbf{G}}|\rho_{\mathbf{G}}|^2 + b_T \sum_{\mathbf{G}_1+\mathbf{G}_2+\mathbf{G}_3=0} \rho_{\mathbf{G}_1}\rho_{\mathbf{G}_2}\rho_{\mathbf{G}_3} + O(\rho^4).$$

V. N. Ryzhov and E. E. Tareyeva, Phys. Rev. B 51, 8789 (1995); Physica A 314, 396-404 (2002); Physica A 432, 279–286 (2015).

The first term in expansion is the free energy of a deformed solid

$$H_E = \frac{1}{2}\int d^2r \left[2\mu u_{ij}^2 + \lambda u_{kk}^2\right], \qquad u_{ij} = \frac{1}{2}\left[\frac{\partial u_i(\mathbf{r})}{\partial r_j} + \frac{\partial u_j(\mathbf{r})}{\partial r_i}\right]$$

The singular part of the displacement field corresponds to dislocations and disclinations

Melting scenarios in two-dimensions: Landau and BKTHNY theories

$$F = \frac{1}{2}\int \sum_{\mathbf{G}} \left[A|\mathbf{G}\times\nabla\rho_{\mathbf{G}}|^2 + B|\mathbf{G}\cdot\nabla\rho_{\mathbf{G}}|^2 + C|\rho_{\mathbf{G}}(\mathbf{G}\cdot\nabla)\rho_{\mathbf{G}}|\right] d^2r +$$

$$+\frac{1}{2}a_T\sum_{\mathbf{G}}|\rho_{\mathbf{G}}|^2 + b_T\sum_{\mathbf{G}_1+\mathbf{G}_2+\mathbf{G}_3=0}\rho_{\mathbf{G}_1}\rho_{\mathbf{G}_2}\rho_{\mathbf{G}_3} + O(\rho^4).$$

Dislocation unbinding temperature T_m.
The modulus of the order parameter vanishes at temperature T_{MF} if the free energies of the liquid and solid phases are equal.

There are two possibilities:

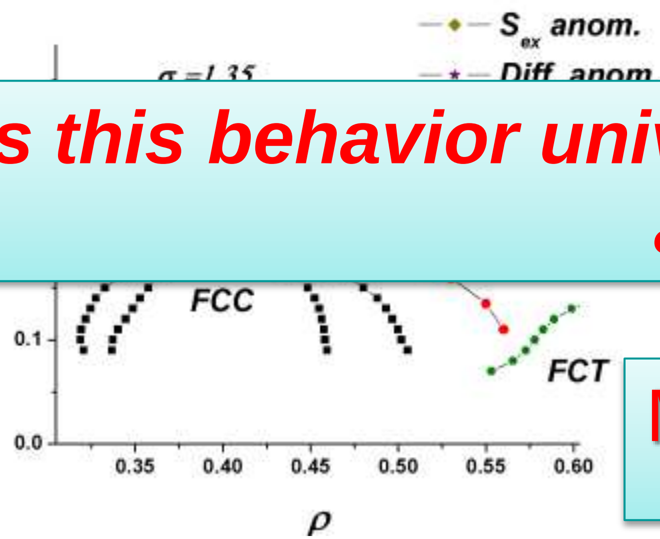
1: $T_m < T_{MF}$. The system melts via two continuous transitions of the Kosterlitz–Thouless type with the unbinding of dislocation pairs.
2: $T_m > T_{MF}$. The system melts via a first-order transition because of the existence of third-order terms in the Landau expansion.

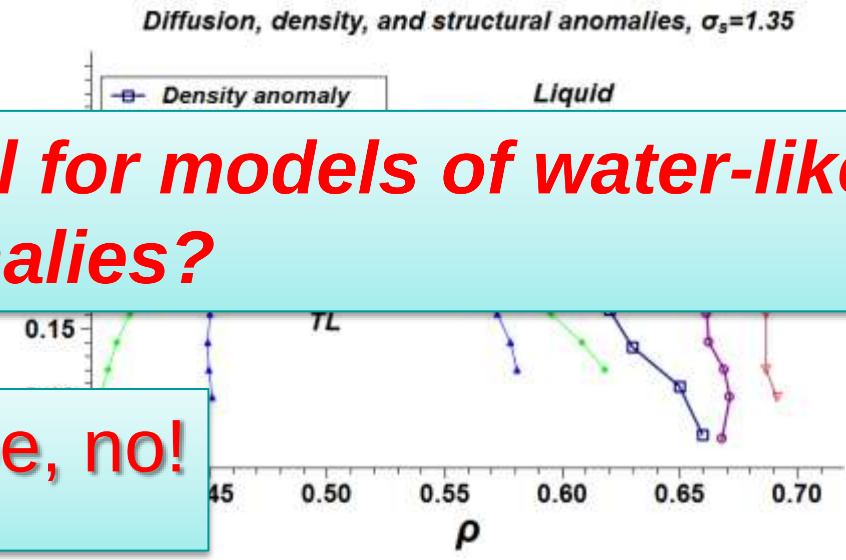
Possible scenarios: grain boundaries (S.T. Chui, Phys. Rev. Lett. 48, 933 (1982); Phys. Rev. B 28, 178 (1983)); dissociation of disclination quadrupoles (V.N. Ryzhov, Zh. Eksp. Theor. Phys. 100, 1627 (1991)), etc…

Anomalous behavior of the core-softened system in 2D: sequence of anomalies in core-softened systems

3D *(Yu. D. Fomin, E. N. Tsiok, and V. N. Ryzhov, J. Chem. Phys. 135, 234502 (2011); Yu. D. Fomin, E. N. Tsiok, and V. N. Ryzhov, Phys. Rev. E 87, 042122 (2013))*

2D (*Inversion of sequence of diffusion and structural anomalies in core-softened systems D.E. Dudalov, Yu.D. Fomin, E.N. Tsiok, and V.N. Ryzhov, Soft Matter 10, 4966 (2014))**)*





Is this behavior universal for models of water-like anomalies?

May be, no!

Waterlike sequence of anomalies (J.R. Errington, P.D. Debenedetti, Nature (London) 409 (2001) 318)

Silicalike sequence of anomalies (S. Shell, P.G. Debenedetti, and A.Z. Panagiotopoulos, Phys. Rev. E ***66****, 011202 (2002); Yu. D. Fomin, E. N. Tsiok, and V. N. Ryzhov, Phys. Rev. E 87, 042122 (2013))*

Melting of soft disks (S.C. Kapfer and W. Krauth, Phys. Rev. Lett. 114, 035702 (2015))