Nuclear "pasta" phases by Quantum Molecular Dynamics

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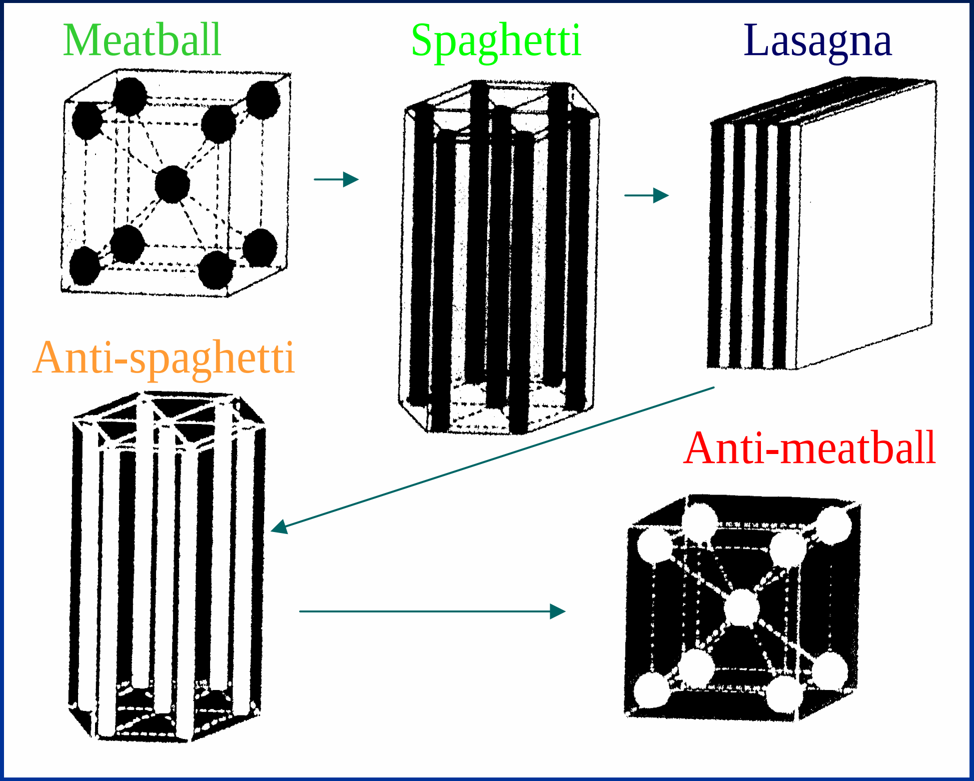
Nuclear Pasta Structure



Oyamatsu,93

With increasing matter density, the shape of nuclei changes from sphere to cylinder, slab, cylindrical bubble and spherical bubble, successively, and eventually becomes homogeneous nuclear matter. (Ravenhall et al.,83, Hashimoto et al, 84,)

Essentially this change is described by the surface energy

$$g \equiv \frac{surfacearea}{(volume)^{2/3}}$$

minimum principle.

Meatball
Spaghetti
Lasagna
Anti-spaghetti
Anti-meatball
→"Pasta" Phases

Nuclear Pasta Structure

- Liquid drop model

  Ravenhall et al., 83,Hashimoto et al, 84, Oyamatsu et al., 84,………

  Watanabe et al., 00, and 01, Iida et al.,01 ………Oyamatsu & Iida (06,)

  stability and fluctuations analysis with the analogy of liquid crystal

  Pethick, Potekhin,98, Watanabe et al., 00, ….

- QMD (Quantum Molecular Dynamics) method

  Maruyama, 98, Watanabe et al., 01,……06, Sonoda et al. 07

- Conventional MD Horowitz et al 04, …………..,05

  complementary, large volume and large particles simulations are possible.

We improved Maruyama method and succeeded to construct the pasta structure by QMD.

QMD is very suitable method for studying **Nuclear Pasta Structure.**

- No assumptions on nuclear shapes, since nuclear system is treated in degrees of freedom of nucleons.
- Thermal fluctuations are necessarily included.

Quantum Molecular Dynamics

- Model Hamiltonian 1 (Chikazumi *et al* Phys.Rev.C 63 024602(2001))

$$\mathcal{H} = \sum_i \frac{P_i^2}{2m_i} + V_{\mathrm{Pauli}} + V_{\mathrm{Skyrme}} + V_{\mathrm{sym}} + \boxed{V_{\mathrm{surface}}} + V_{\mathrm{MD}} + V_{\mathrm{Coulomb}}$$

Kinetic Energy | Pauli Potential | Nuclear Force | Coulomb Energy

The surface term, which depends on the density gradient, is added to the original Maruyama model in order to make the surface of nuclei smooth. In the original model, the surface of large nuclei are slightly bumpy.

- Model Hamiltonian 2 (Maruyama *et al* Phys.Rev.C 57 655(1998))

The original model without the surface term.

Equations of Model Hamiltonian 1

$$\mathcal{H} = \sum_i \frac{\boldsymbol{P}_i^2}{2m_i} + V_{\text{Pauli}} + V_{\text{Skyrme}} + V_{\text{sym}} + V_{\text{surface}} + V_{\text{MD}} + V_{\text{Coulomb}}$$

(Chikazumi *et al* Phys.Rev.C 63 024602(2001)

Definition of densities

$$\begin{aligned}
\langle \rho_i \rangle &\equiv \sum_{j(\neq i)} \rho_{ij} \equiv \sum_{j(\neq i)} \int d^3\boldsymbol{r}\, \rho_i(\boldsymbol{r}) \rho_j(\boldsymbol{r}) \\
\langle \tilde{\rho}_i \rangle &\equiv \sum_{j(\neq i)} \tilde{\rho}_{ij} \equiv \sum_{j(\neq i)} \int d^3\boldsymbol{r}\, \tilde{\rho}_i(\boldsymbol{r}) \tilde{\rho}_j(\boldsymbol{r}) \\
\rho_i(\boldsymbol{r}) &= \frac{1}{(2\pi L)^{3/2}} \exp\left\{ -\frac{1}{2L} (\boldsymbol{r} - \boldsymbol{R}_i)^2 \right\} \\
\tilde{\rho}_i &= \frac{1}{(2\pi \tilde{L})^{3/2}} \exp\left\{ -\frac{1}{2\tilde{L}} (\boldsymbol{r} - \boldsymbol{R}_i)^2 \right\} \\
& L = 1.95\text{fm}^2, \tau = 1.33333, \tilde{L} = \frac{(1+\tau)^{1/\tau}}{2} L
\end{aligned}$$

Pauli potential

$$\begin{aligned}
V_{\text{Pauli}} &= \frac{C_p}{2(q_0 p_0/\hbar c)^3} \sum_{i,j(\neq i)} \exp\left[-\frac{|\boldsymbol{R}_i - \boldsymbol{R}_j|^2}{2q_0^2} - \frac{|\boldsymbol{P}_i - \boldsymbol{P}_j|^2}{2p_0^2} \right] \delta_{\tau_i \tau_j} \delta_{\sigma_i \sigma_j} \\
& C_P = 115.0\text{MeV}, p_0 = 120.0\text{MeV}, q_0 = 2.5\text{fm} \\
& \tau_i : \text{isospin}, \sigma_i : \text{spin}
\end{aligned}$$

Skyrme potential

$$V_{\text{Skyrme}} = \frac{\alpha}{2\rho_0}\sum_i <\rho_i> + \frac{\beta}{(1+\tau)\rho_0^{\tau}}\sum_i <\tilde{\rho}_i>^{\tau}$$

$$\alpha = -121.9\text{MeV}, \beta = 197.3\text{MeV}$$

Symmetry potential

$$V_{\text{sym}} = \frac{C_{s0}}{2\rho_0}\sum_{i,j(\neq i)}(1-2|c_i-c_j|)\rho_{ij}$$

$$C_{s0} = 25.0\text{MeV}, c_i : \text{isospin}$$

Surface potential

$$V_{\text{surface}} = \frac{V_{\text{SF}}}{2\rho_0^{5/3}}\sum_{i,j(\neq i)}\int d^3\boldsymbol{r}\boldsymbol{\nabla}\rho_i(\boldsymbol{r})\boldsymbol{\nabla}\rho_j(\boldsymbol{r})$$

$$V_{SF} = 20.68\text{MeV}$$

Momentum dependent potential

$$V_{\text{MD}} = \frac{C_{\text{ex}}^{(1)}}{2\rho_0}\sum_{i,j(\neq i)}\frac{1}{1+\left(\frac{|\boldsymbol{P}_i-\boldsymbol{P}_j|}{\mu_1\hbar}\right)^2}\rho_{ij} + \frac{C_{\text{ex}}^{(2)}}{2\rho_0}\sum_{i,j(\neq i)}\frac{1}{1+\left(\frac{|\boldsymbol{P}_i-\boldsymbol{P}_j|}{\mu_2\hbar}\right)^2}\rho_{ij}$$

$$C_{ex(1)} = -258.5\text{MeV}, C_{ex(2)} = 375.6\text{MeV},$$

$$\mu_1 = 2.35\text{MeV}, \mu_2 = 0.4\text{MeV}$$

Coulomb potential

$$V_{\text{Coulomb}} = \frac{e^2}{2}\sum_{i,j(\neq i)}\left(\tau_i+\frac{1}{2}\right)\left(\tau_j+\frac{1}{2}\right)\int\int d^3\boldsymbol{r}d^3\boldsymbol{r}'\frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|}\rho_i(\boldsymbol{r})\rho_j(\boldsymbol{r}')$$

- **These Hamiltonians include free parameters, 14 in Model 1 , and 13 in Model 2.**

- The values of these parameters are determined to reproduce
  the saturation properties of symmetric nuclear matter, and
  the binding energy and rms radius of stable nuclei.

Simulation settings

Eq. Motion of nucleons in QMD

$$\dot{\mathrm{R}}_i = \frac{\partial \mathcal{H}}{\partial \mathrm{P}_i} - \xi_R \frac{\partial \mathcal{H}}{\partial \mathrm{R}_i},$$

$$\dot{\mathrm{P}}_i = -\frac{\partial \mathcal{H}}{\partial \mathrm{R}_i} - \xi_P \frac{\partial \mathcal{H}}{\partial \mathrm{P}_i}.$$

Ground state is obtained by cooling of hot matter by frictional relaxation,

the time scale of the cooling ~O(1,000—10,000) fm/c,

much larger than

$$\tau_{\text{relax}} \equiv \frac{\text{length scale of inhomogeneity}}{\text{sound velocity}} \sim \frac{10\text{fm}}{0.1c} \sim 100\text{fm}/c$$

Simulation Settings

2,048 or 10,976 nucleons in simulation box.
Periodic boundary condition.
Proton fraction x= n/(p+n) =0.3.

Computation: RSCC (RIKEN Super Combined Cluster) with

MD GRAPE (the pipeline processing module for calculating the forces between particles, originally developed for the gravitational N-body problem)

CPU time to get one model ; 2 ~ 3 weeks for spherical cases (lower density cases)

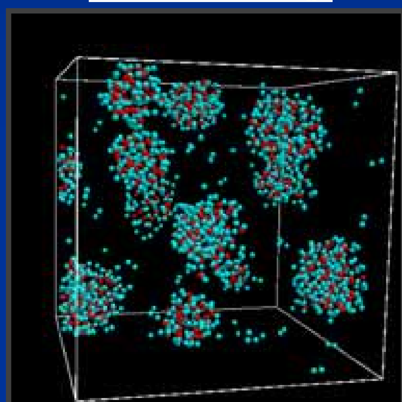
1. ~ 1.5 months for Spaghetti and Lasagna phases (higher cases).

Pasta at zero temperature

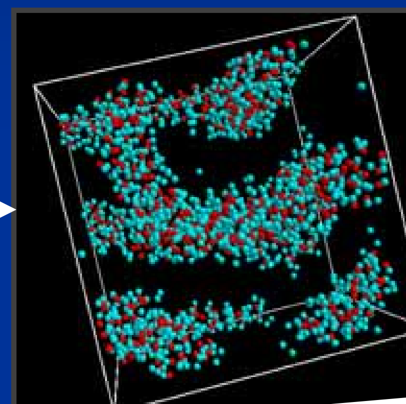
Cooling of hot nuclear matter (~10 MeV) below 0.1 MeV

Model 1

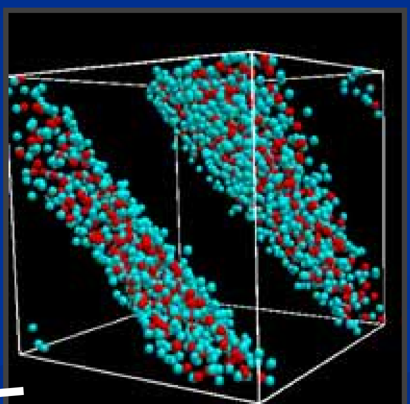
Sphere $0.100\ \rho_0$

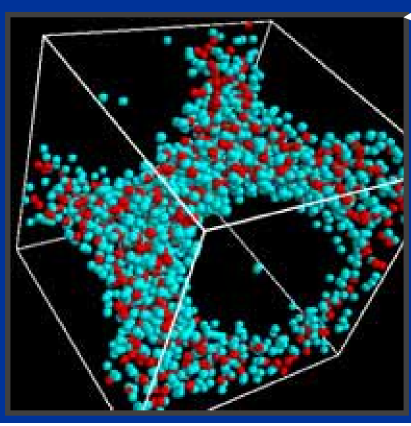


cylinder $0.200\ \rho_0$

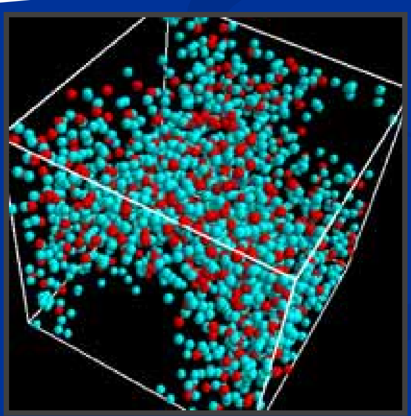


Slab $0.393\ \rho_0$





cylinder-like Holes $0.490\ \rho_0$



Spherical Holes $0.575\ \rho_0$

Red : Protons

Blue: Neutrons

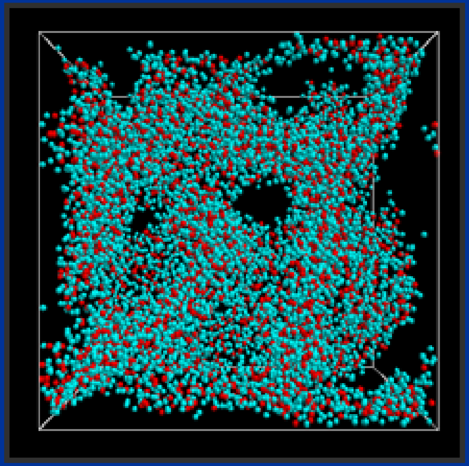
ρ_0 =0.168 fm^{-3}

(Nuclear density)

Sponge-like Structure

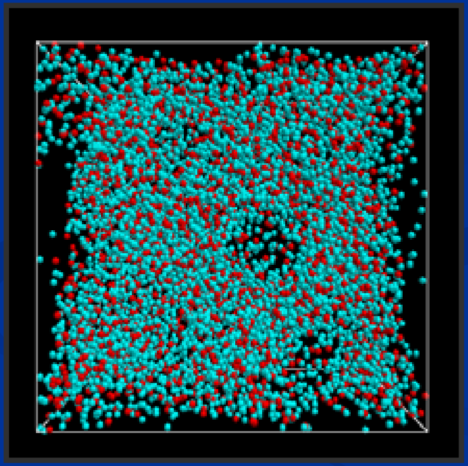
Between cylinder and slab, slab and cylinder-like holes
Multiply connected “Sponge-like” structure appears

Between cylider and slab



10976 nucleons at 0.3 ρ_0

Between slab and cylinder holes



10976 nucleons at 0.45 ρ_0

These intermediate phases at least meta-stable

Minkowski Functionals

— A powerful tool for morphological analysis —

Euler characteristic

$$\chi = \frac{1}{2\pi}\int_{\partial} G\,dA$$

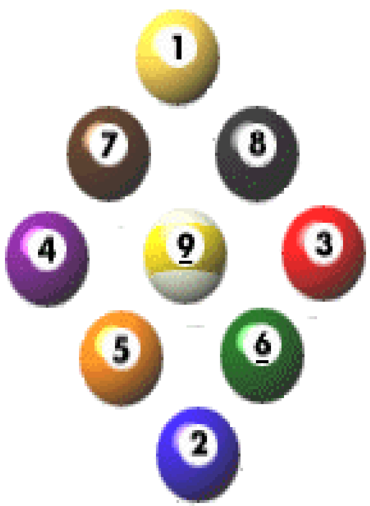
χ = (number of isolated regions) – (number of tunnels) + (number of cavities)

About a surface of a body K in 3D space

$$\text{mean curvature} \quad H = (\kappa_1 + \kappa_2)/2$$

$$\text{Gaussian curvature} \quad G = \kappa_1 \kappa_2$$

κ_1, κ_2 : principal curvatures



$$\chi = 9$$

$$\chi = 3 - 3 = 0$$

$$\chi = 1 - 5 = -4$$

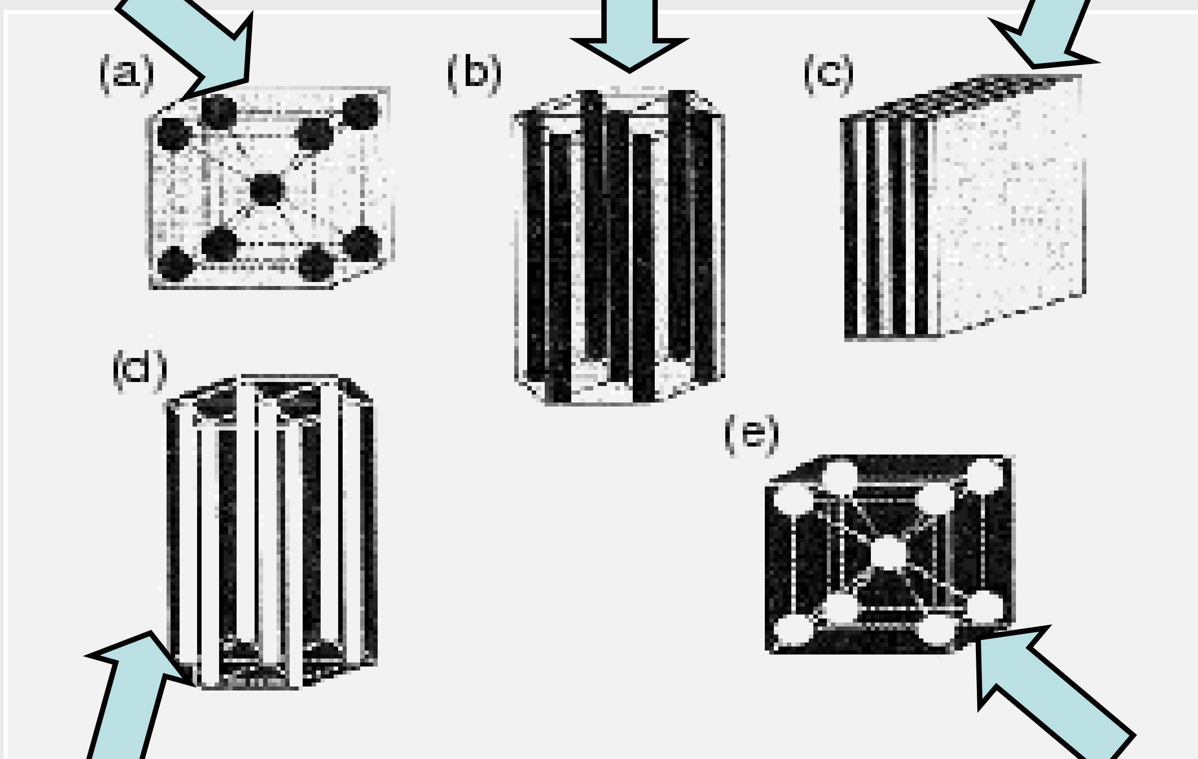
Figures from a Hikage slide

Pasta phases are discriminated by H and χ.

SP:H>0, χ >0

C:H>0, χ =0

S:H=0, χ =0



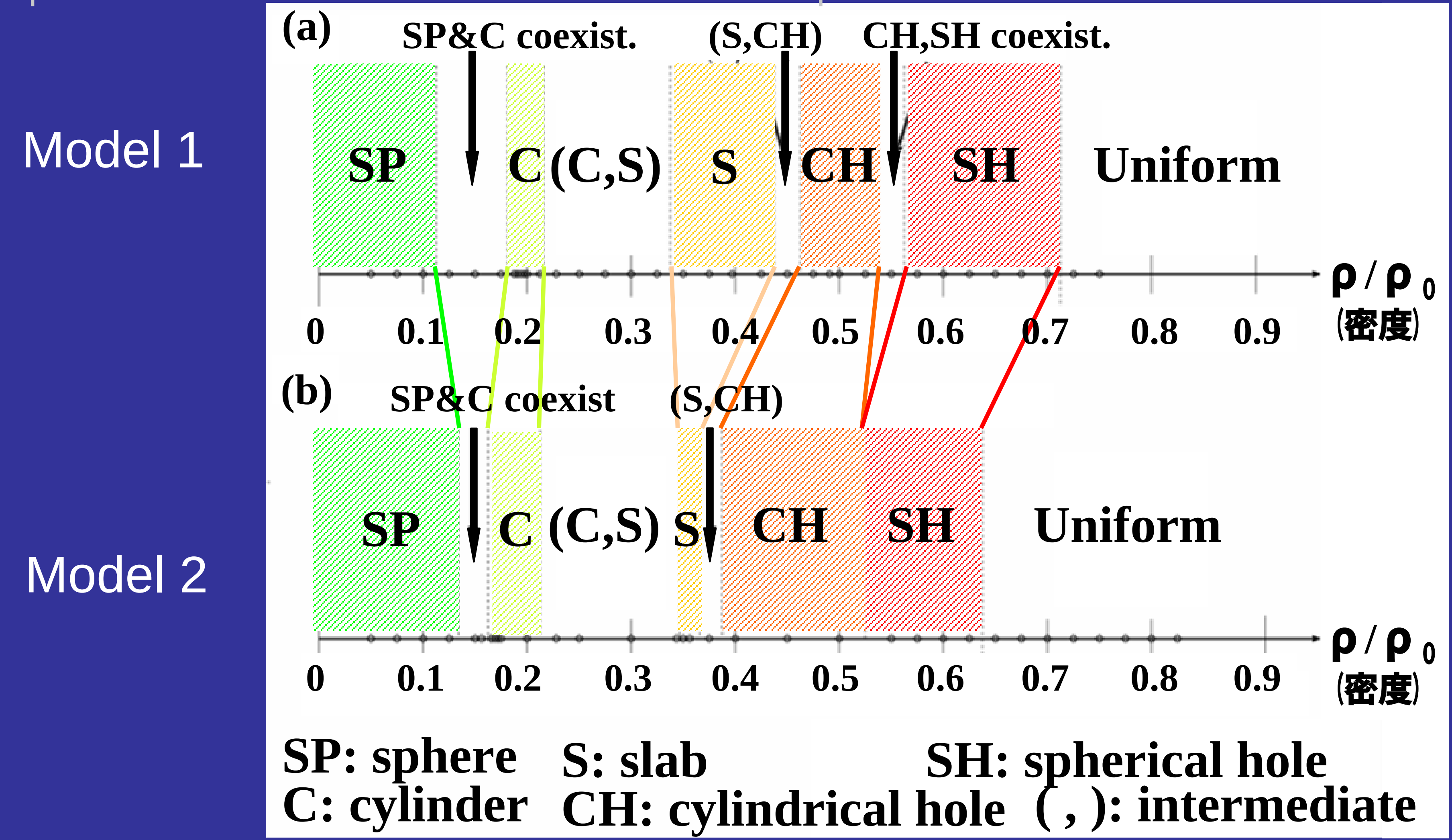
CH:H<0, χ =0

SH:H<0, χ >0

χ <0 ・・・ Sponge-like Structure

Phase diagram at zero temperature

Sphere →Rod → Slab → Rod-like bubbles → Spherical bubbles →Uniform matter



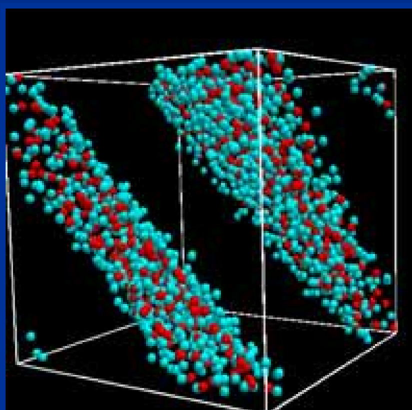
Melting density of the pasta in Model 1 is 0.7 nuclear density, higher than that of Model 2, 0.65 nuclear density by the effect of surface term.

Pasta at finite temperatures

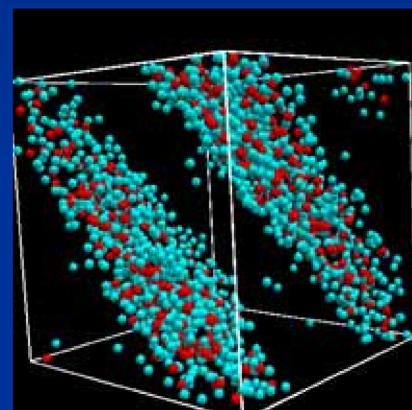
Model 1

0.393 ρ_0 (Slab nuclei at zero temperature)

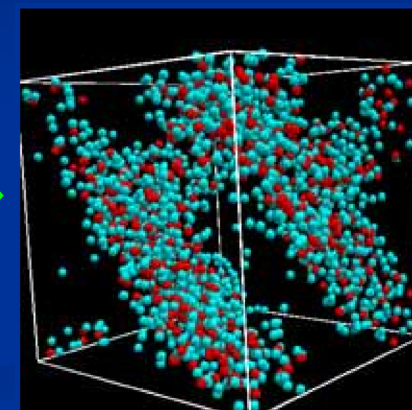
T= 0 MeV



T= 1 MeV



T= 2 MeV



Slab Nuclei

Evaporated Neutrons

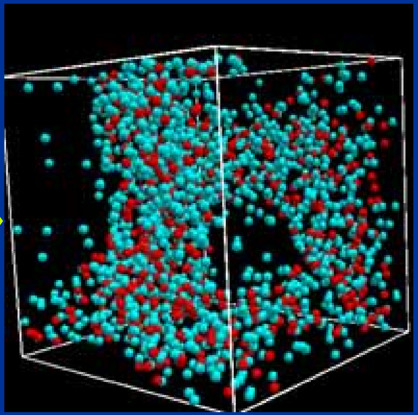
Connected Slab

dripped neutrons Increases

nuclear surfaces become more diffusive

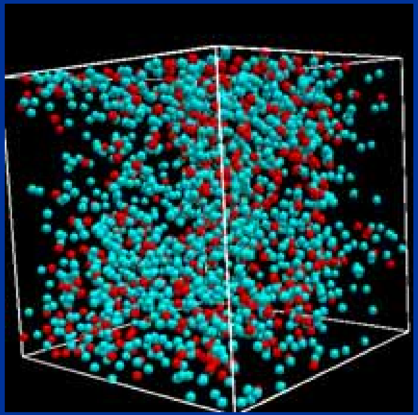
Pasta at finite temperature

T=3MeV



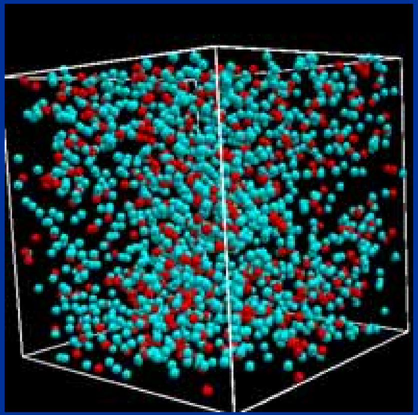
cylindrical hole-like structure

T=5MeV



Cannot identify nuclear surface

T=6MeV

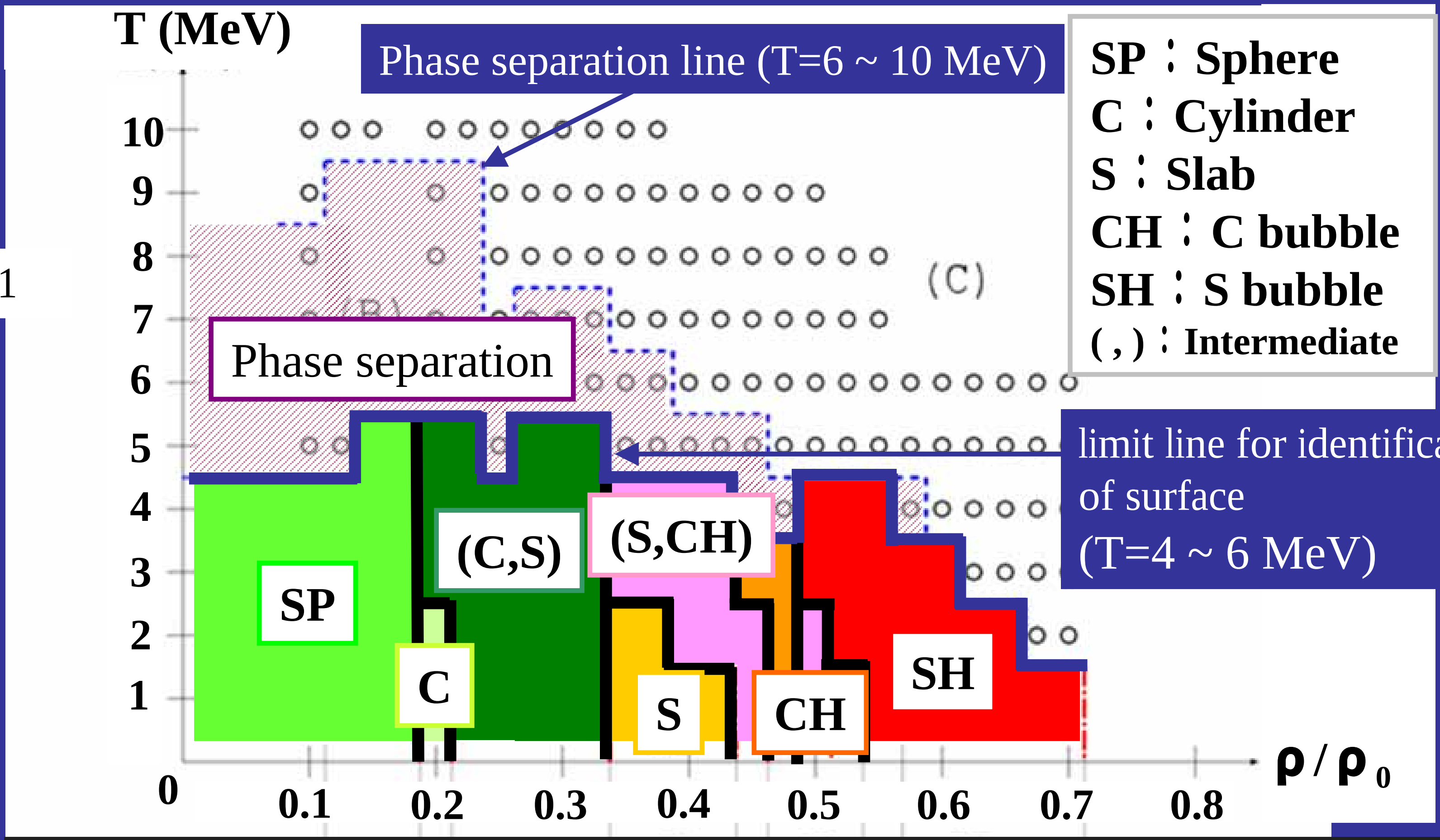


Phase separation disappears

Phase transition, Melting surface, Dripped protons, Disappearance of phase separation occur successively

Phase diagram at finite temperatures

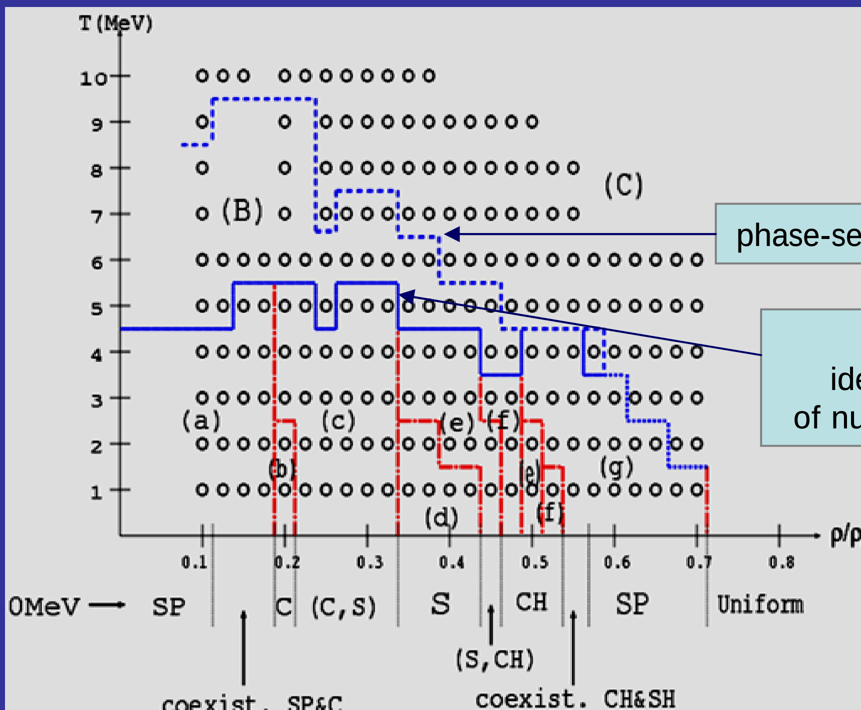
Model 1



Thermal fluctuation increases volume fraction of nuclei.
Above T= 4 ~ 6 MeV, cannot identify surface.
At T= 6 ~ 10 MeV, Liquid-gas phase separation.

Comparison of Phase diagrams between two models

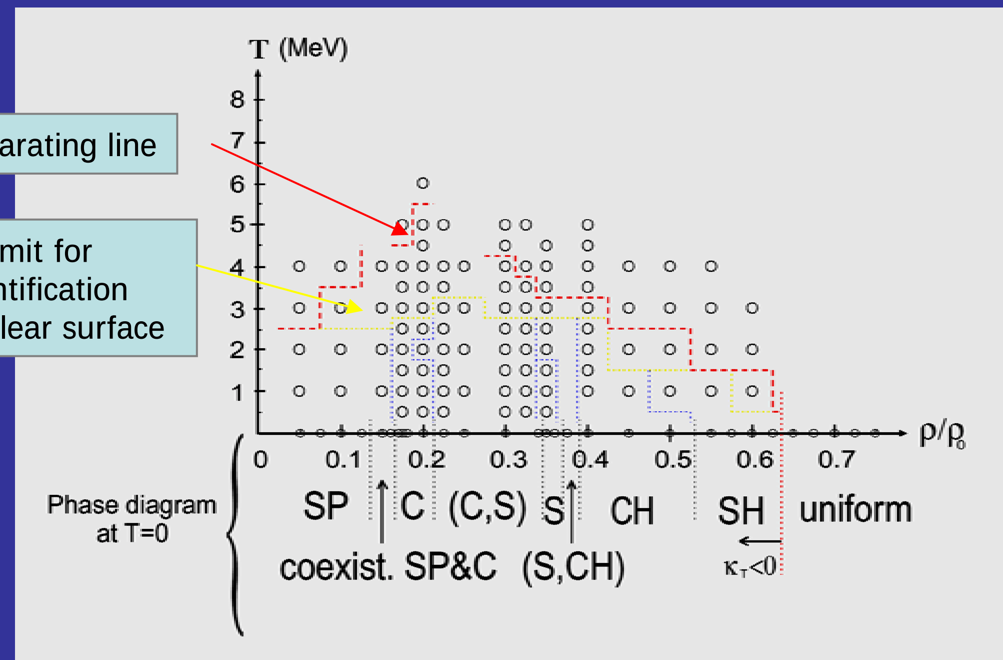
Model 1



phase-separating line

limit for identification of nuclear surface

Model 2



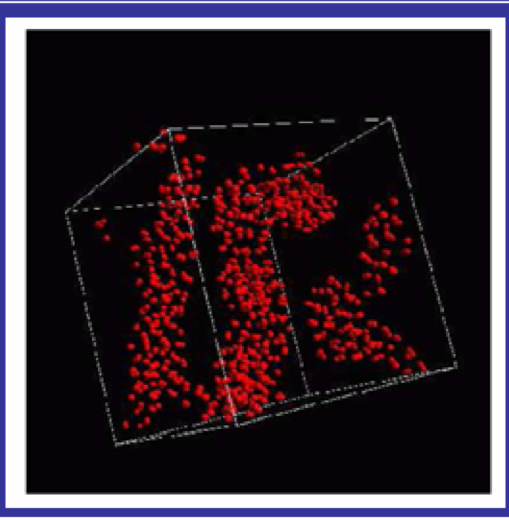
Nuclear pasta remains in higher temperature in Model 1 :

limit for identification of nuclear surface: T=4 ~ 6 MeV (Model 1), 2 ~ 3MeV (Model 2)

Phase separation line: T=6 ~ 10 MeV ,3 ~ 5MeV

Case of X=p/(p+n)=0.1, Model 2

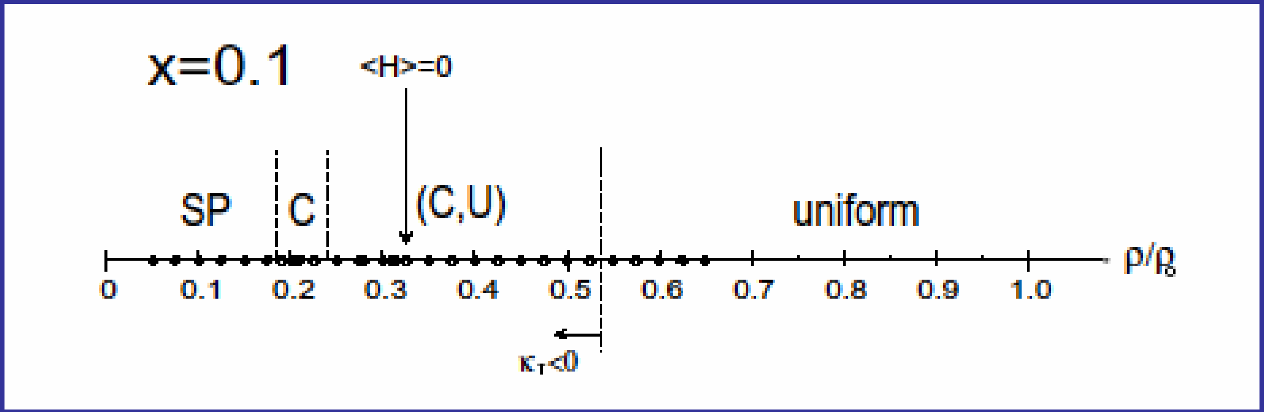
(deep side of inner crust of neutron stars)



The proton distribution of cylinder phase at $\rho = 0.2\rho_0$ and T=0.1MeV.

Neutrons which spread over the whole space are not depicted in this figure.

Phase diagram



Spherical and cylindrical phase are only observed in 0.18- 0.53 ρ_0 .

No pasta phases are observed in densities higher than 0.53 ρ_0

More systematic survey of the nuclear pasta phases of x=0.1 is under progress.

Neutrino Opacity of Pasta Phases

Sonoda et al PR C, 2007

Neutrino transport
--- a key element for success of supernovae

- Neutrinos are trapped in collapsing phase by coherent scattering with nuclei (K.Sato,75) Lepton fraction , Y_{lep}, affects EOS.

How pasta phases change neutrino transport in collapsing cores ?
Pioneering investigation were done by Horowitz group (04,….).

Neutrino cross section of neutrino-Pasta

Cross section of neutrino-nucleon system due to coherent scattering

$$\frac{1}{N}\frac{d\sigma}{d\Omega}(\mathbf{q}) = \boxed{\frac{G_F^2 E_\nu^2}{4\pi^2}(1+\cos\theta)\cdot c_v^{(n)2}} \times \boxed{\overline{S}(\mathbf{q})}$$

Neutrino-neutron cross section

Amplification factor
(Static structure factor)

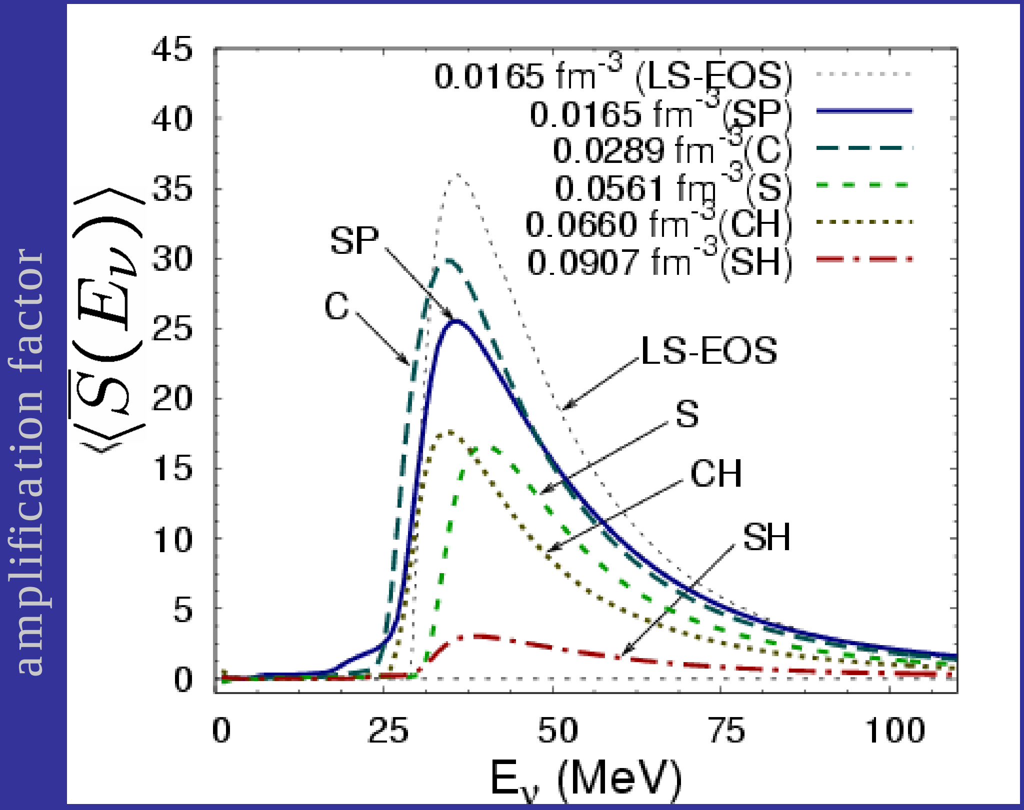
Because collapsing cores are poly-crystalline, the opacity would be well characterized by the angle-average of $\overline{S(q)}$.

Total transport cross section: $\sigma_t = \langle \overline{S}(E_\nu) \rangle \sigma_t^0$ $\qquad \sigma_t^0 = \frac{2G_F^2 E_\nu^2}{3\pi} c_\nu^{(n)2}$

$\langle \overline{S}(E_\nu) \rangle$ → Angle-averaged amplification factor by pasta structure

QMD results : change of the amplification factors with increasing density

Y_e=0.3, T=1 MeV



Neutrino energy

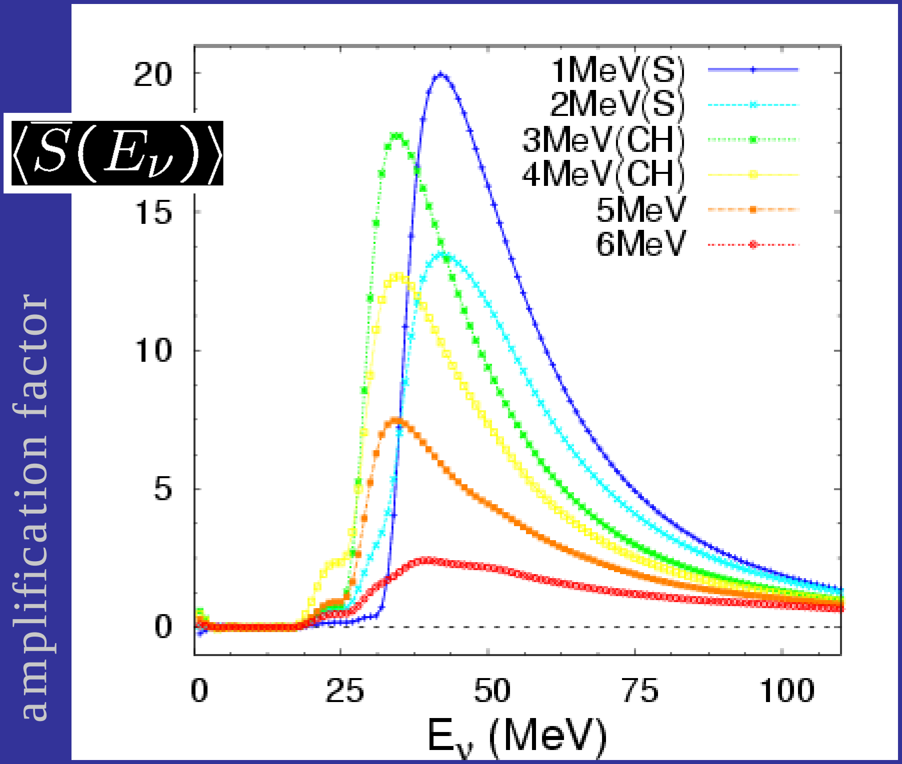
Compared with the Lattimer- Swesty model (LS-EOS),

- the energy of peaks are lower, and
- the width of peaks are wider,

due to lattice disorder and irregularity of nuclei.

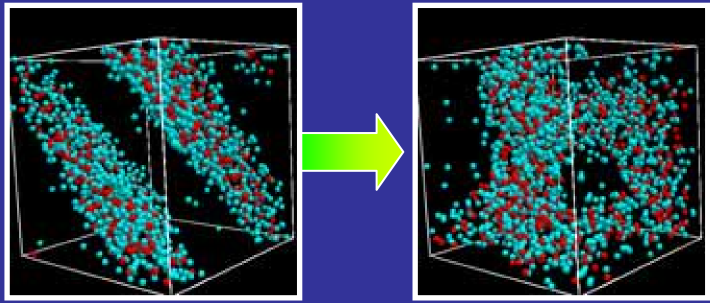
QMD results: change of the amplification factors with increasing density

Y_e=0.3, **ρ** =0.0660fm^{-3} (Slab at T=0)



Neutrino energy

T= 1 MeV **T= 3 MeV**



- Peak is lowered and broader by increasing temperature due to lattice disorder and Irregularity of nuclei.
- Transition from slab(2MeV) to rod-like bubbles(3MeV) dramatically changes peak energy lower ,and peak height higher.

Difficult to discuss the effects on supernova explosion at present stage.

Summery

- Vivid pictures of nuclear pasta structure were obtained by QMD simulations.
- Difference of phase diagrams of two models available at present was investigated, but ambiguity on the dependence on nuclear potentials still remains.
- Neutrino opacity of the pasta phases described well by QMD were calculated.
- More systematic survey is under progress.