Electrostatic energy of Coulomb crystals with polarized electron background

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At zero temperature the type of the lattice is mainly determined by electrostatic energy (all ions are in equilibrium positions $\mathbf{R}_l$). So we should consider different lattices, calculate their electrostatic energies and find out which is more preferable. For description electron background polarisation effects we use three dielectric function (for simplicity we call them "models").

Crystal with uniform electron background

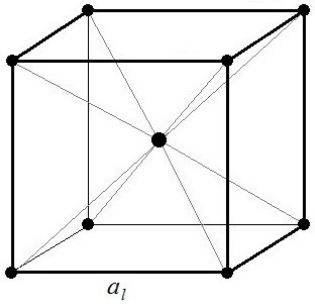
$$U_{\mathrm{M}} = \sum_{i=1}^{N}\sum_{j=1}^{i-1}\frac{Z_i Z_j e^2}{|\mathbf{R}_i - \mathbf{R}_j|} - n_e \sum_{i=1}^{N} Z_i e^2 \int_V \frac{\mathrm{d}\mathbf{r}}{|\mathbf{R}_i - \mathbf{r}|} + \frac{n_e^2}{2}\int_V\int_V \frac{e^2 \mathrm{d}\mathbf{r}\mathrm{d}\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|}$$

$$U_{\mathrm{M}} = N\frac{Z^2 e^2}{a}\zeta, \qquad a \text{ is ion sphere radius}$$

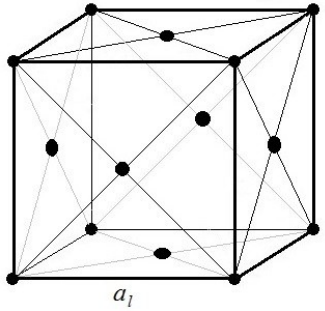
$$\zeta = \frac{a}{2N_{\mathrm{cell}}}\sum_{lpp'}(1-\delta_{pp'}\delta_{\mathbf{R}_l 0})\frac{\mathrm{erfc}\,(AY_{lpp'})}{Y_{lpp'}} - \frac{Aa}{\sqrt{\pi}} - \frac{3}{8A^2a^2}$$

$$+\frac{3}{2N_{\mathrm{cell}}^2 a^2}\sum_{mpp'}(1-\delta_{\mathbf{G}_m 0})\frac{1}{G_m^2}\exp\left[-\frac{G_m^2}{4A^2} + i\mathbf{G}_m(\boldsymbol{\chi}_p - \boldsymbol{\chi}_{p'})\right].$$

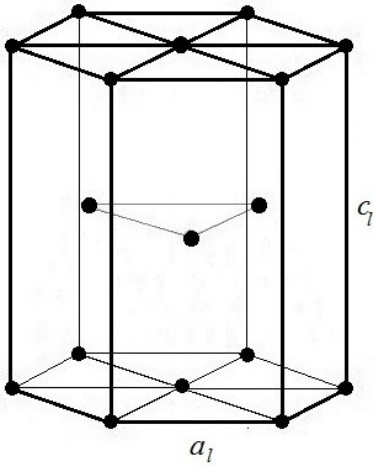
ζ — Madelung constant



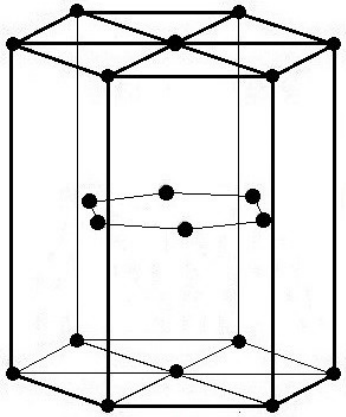
BCC lattice $\zeta = -0.895929255682$



FCC lattice $\zeta = -0.895873615195$



HCP lattice $\zeta = -0.895838120459$



MgB_2 lattice $\zeta = -0.89450562823$

In their lowest energy state the nuclei form a body centred cubic lattice[7,8]

Ruderman M. (1968) "Crystallization and Torsional Oscillations of Superdense Stars"

Crystal with polarized electron background

the static longitudinal dielectric function $\epsilon(q)$

$$\epsilon(q) = 1 + \frac{\kappa_{\rm TF}^2}{q^2}\epsilon_2(q)$$

$$\kappa_{\rm TF} a = 0.1850\, Z^{1/3}\, \frac{(1+x^2)^{1/4}}{x^{1/2}}$$

x is the relativistic parameter of the electron

$$x \equiv \frac{p_{\rm F}}{m_e c} \approx 0.01 \left(\rho \frac{Z}{A}\right)^{1/3}$$

$$\epsilon_{2{\rm J}}(q) = \frac{2}{3} - \frac{2}{3}\frac{y^2 x}{\gamma}\ln\left(x+\gamma\right) + \frac{x^2+1-3x^2y^2}{6yx^2}\ln\left|\frac{1+y}{1-y}\right| + \frac{2y^2x^2-1}{6yx^2}\frac{\sqrt{1+x^2y^2}}{\gamma}\ln\left|\frac{y\gamma+\sqrt{1+x^2y^2}}{y\gamma-\sqrt{1+x^2y^2}}\right|$$

where $y = \hbar q/(2p_{\rm F}) \approx 0.26 q a Z^{-1/3}$ and $\gamma \equiv \sqrt{1+x^2}$.

Jancovici (J) model

⇨

$$\epsilon_{2{\rm L}}(q) = \frac{1}{2} + \frac{1-y^2}{4y}\ln\left|\frac{1+y}{1-y}\right|$$

Lindhard (L) model

⇨

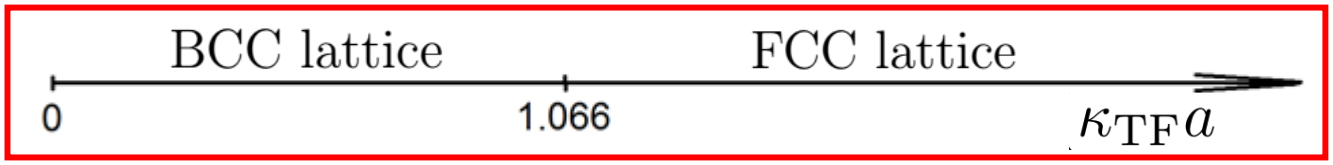
$$\epsilon_{2{\rm TF}}(q) = 1$$

Thomas-Fermi (TF) model

Thomas-Fermi (TF) model U_{TF}

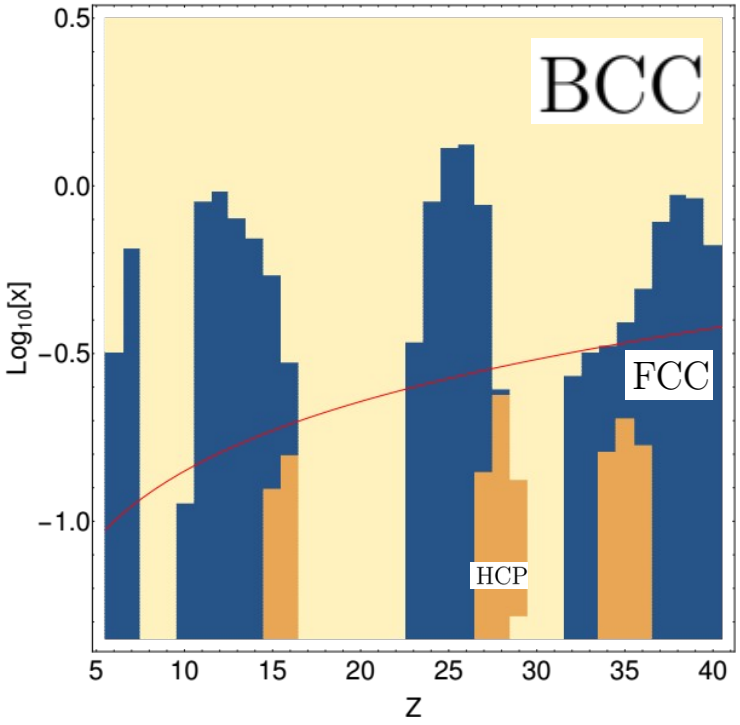
$$U_{\mathrm{TF}} \equiv NZ^2e^2\left\{\frac{1}{N_{\mathrm{cell}}}\sum_{l,p,p'}(1-\delta_{\mathbf{R}_l0}\delta_{pp'})\frac{E_-+E_+}{4Y_l}-\frac{\kappa_{\mathrm{TF}}}{2}\mathrm{erf}\left(\frac{\kappa_{\mathrm{TF}}}{2A}\right)-\frac{2\pi n}{\kappa_{\mathrm{TF}}^2}\right.$$
$$\left.-\frac{A}{\sqrt{\pi}}e^{-\frac{\kappa_{\mathrm{TF}}^2}{4A^2}}+\frac{1}{N_{\mathrm{cell}}^2}\sum_{m,p,p'}\frac{2\pi n}{G_m^2+\kappa_{\mathrm{TF}}^2}\exp\left[-\frac{G_m^2+\kappa_{\mathrm{TF}}^2}{4A^2}-i\mathbf{G}_m(\boldsymbol{\chi}_p-\boldsymbol{\chi}_{p'})\right]\right\},$$

where $E_\pm = \mathrm{e}^{\pm\kappa Y_l}\,\mathrm{erfc}\,(AY_l \pm \kappa_{\mathrm{TF}}/(2A))$, $\mathbf{Y}_l = \mathbf{R}_l + \boldsymbol{\chi}_p - \boldsymbol{\chi}_{p'}$, $\mathrm{erf}(x)$ is the error function, $\mathrm{erfc}(x) \equiv 1-\mathrm{erf}(x)$, and A is an arbitrary constant; $A \approx 2/a$ is most suitable because it gives good numerical convergence of both sums.



The bcc lattice possess the smallest electrostatic energy at $\kappa_{\mathrm{TF}}a < 1.065714$, while at higher $\kappa_{\mathrm{TF}}a$ — the fcc lattice and no other lattice becomes more energetically preferable.

Lindhard (L) model U_{L}



$$U \equiv U_{\mathrm{M}} + \Delta U$$

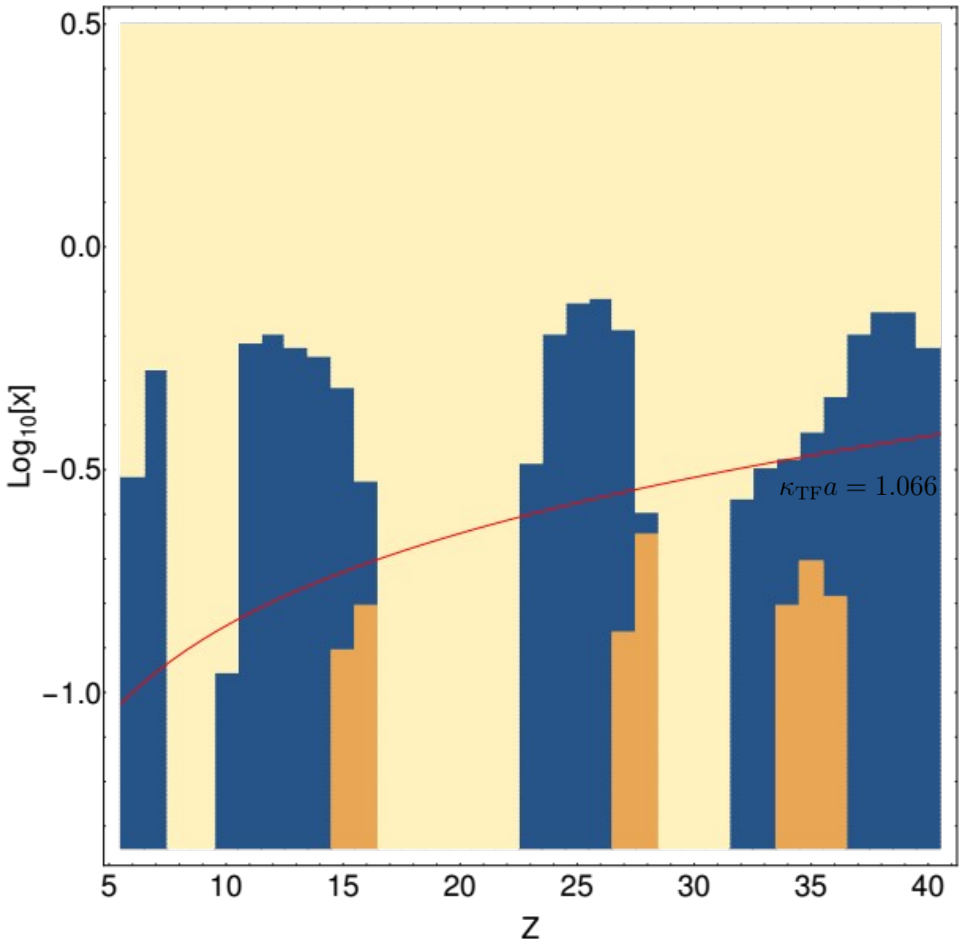
$$\Delta U = N \frac{Z^2 e^2}{a} \frac{3}{2N_{\mathrm{cell}}^2} \times \sum_m{}' \frac{1}{(G_m a)^2} \left[\frac{1}{\epsilon(G_m)} - 1 \right] \sum_{p,p'} e^{i\mathbf{G}_m(\boldsymbol{\chi}_p - \boldsymbol{\chi}_{p'})}$$

$$x \equiv \frac{p_{\mathrm{F}}}{m_e c} \approx 0.01 \left(\rho \frac{Z}{A} \right)^{1/3}$$

At any Z the bcc lattice possesses the lowest U_{L} at $\log_{10}(x) \gtrsim 0.2$ (in other hand, the Lindhard model is valid if $\log_{10}(x) \ll 0$). If we assume that $A = 2Z$ it is equivalent to $\rho \gtrsim 5 \times 10^5$ g cm^{-3}. It means that the most part of the solid neutron star crust has a bcc lattice. The fcc and hcp lattice becomes energetically preferable at lower densities, where this model is mostly not applicable for stars envelopes. Structural transition between lattices is noticeably depends on Z.

Jancovici (J) model U_{J}

The relativistic corrections
to the dielectric function,
which the Jancovici model gives,
do not noticably effect
to the structural transitions
in the Coulomb crystals.



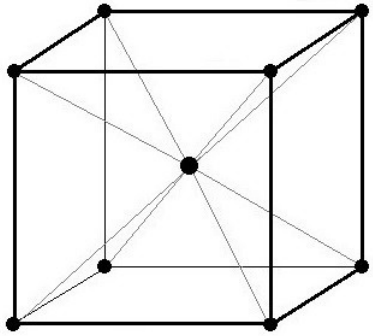
Dusty crystals

ISS "Kulonovskiy Kristall" experiment
shows that dusty (1 μm size) particles
with $Z \sim 3000$ and $\kappa_{\mathrm{D}} a = 0.5 - 3$
form an ordered system
with the hcp and fcc structures.

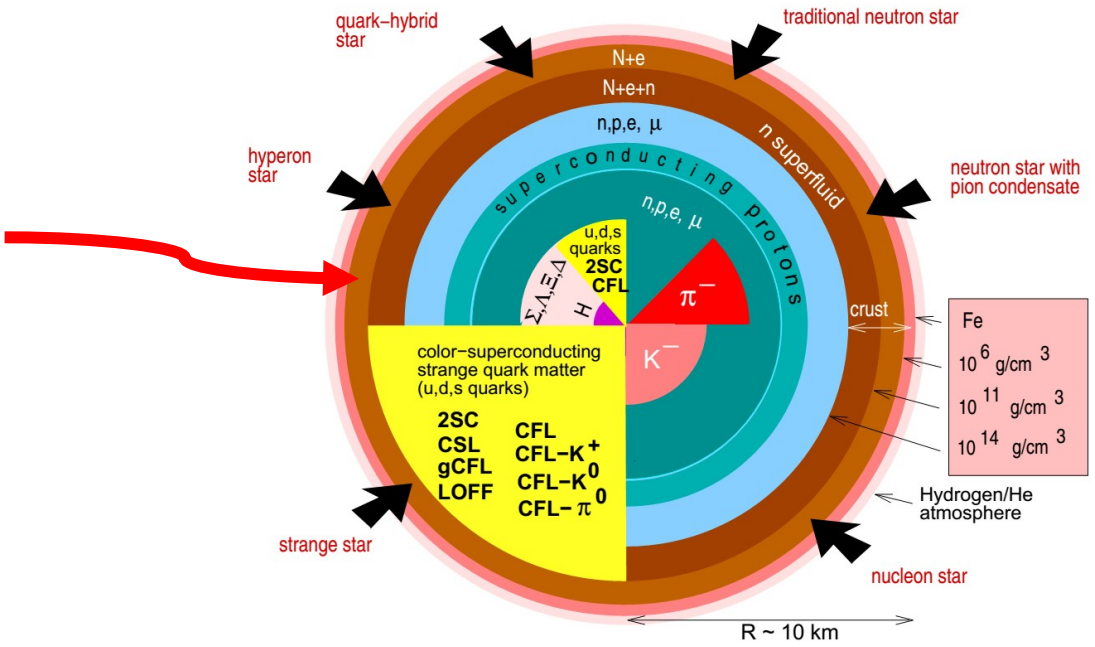
The electrostatic energy of the Coulomb crystal with the Thomas-Fermi dielectric function and the electrostatic energy of the dusty crystal describes by the same equation. Hence the both crystals have the same structural transitions. The difference between them that in the first case background is degenerated (we use $\kappa_{\mathrm{TF}} a$), while in the second case — not (we use $\kappa_{\mathrm{D}} a$). So while the Lindhard model bring us to the fact that at $\kappa_{\mathrm{TF}} a \gtrsim 1$ the fcc and hcp lattice becomes more energetically preferable and the strong dependence structural transitions on Z appears, we can expect a similar situation if higher order corrections to Yukawa crystal are taken into account. Since in dusty systems it is impossible to maintain strictly the same charge for all grains the formation of the hcp-fcc crystal mixture is more likely.

The ground state of the OCP of ions corresponds to the body-centered cubic (bcc) lattice.

Haensel, Potekhin, Yakovlev 2007



$$\rho \gtrsim 10^6 \text{ g cm}^{-3}$$



Weber 2004

Highly likely at $\rho \lesssim 10^6$ g cm^{-3} the neutron star crust is a polycrystal mixture of different lattices or even amorphous solid.