

Liquid-phase epitaxy of neutron star crust and white dwarf core D. A. Baiko



07/12/2023

I. Epitaxy II. Applications Part I: Epitaxy = Epi + taxis = on + arrangement

Neutron Stars (NS) and White Dwarfs (WD)

- Compact stars
- No thermonuclear reactions
- Pressure of degenerate fermions (electrons or neutrons)
- $M \sim M_{\odot}$; $R \sim 10$ km (NS); ~planet Earth (WD)
- $\rho < 10^{15} \text{ g/cm}^3 \text{ (NS)}; \rho < 10^{10} \text{ g/cm}^3 \text{ (WD)}$
- Plasma of fully ionized atoms (nuclei) with uniform degenerate electron background
- Nuclei form strongly non-ideal plasma (liquid)
- As a star cools, the ion liquid crystallizes; background doesn't change
- Crystallization front moves from inside the star out

— Consider gradual freezing of a *one-component* ion crystal

— Suppose that the freezing direction is vertical, while the surfaces of simultaneous freezing are horizontal

Previous, already frozen layers create a set of potential maxima and minima characteristic of a particular crystallographic plane (*under assumption that the frozen part of the crystal has a well-defined top plane and that crystal ions are located precisely at the nodes of the bcc lattice*)
Liquid, on average, is uniform, neutral and approximately the same near any crystal plane



Here, vertical distance from ion plane equal to interplane spacing





— Lateral ion positions in a newly freezing layer are determined by the ions of the previous layers in analogy with liquid-phase epitaxial crystal growth or solidification from melt, the processes well-known in solid-state physics and semiconductor industry

— <u>Due to</u> lack of any ion-orientation dependence (typical of covalent bonds), <u>due to</u> long-range almost pure Coulomb forces extending over a major fraction of the elementary cell and capturing an unbound ion, <u>due to</u> a strong pull on ions to settle at a correct height above the already crystallized surface (related to charge neutrality), and <u>due to</u> extremely slow, with plenty of time for anneal, near-equilibrium nature of crystallization in compact stars,

it should be even easier to accomplish epitaxial growth of Coulomb crystals in dense matter than e.g. silicon in Earth laboratories — Lateral positions of ions being added to a growing crystal are fixed by previous layers. Vertical positions of the ions are determined by charge neutrality

— In a freezing star, interplane distances gradually increase tracing n_e decrease, associated with pressure decrease as one moves away from the center

— This results in a formation of elongated (not cubic!) ion crystals

— There is also a similar mechanism of unidirectional crystal contraction

— The typical length-scale of n_e variation is of the order of the pressure scale height

$$\frac{n_{\rm e}}{\nabla n_{\rm e}} = \frac{4}{3}h_P = \frac{4P_{\rm e}}{3\rho g} = \frac{4}{3}\left(\frac{3Z}{A}\right)^{4/3} \left(\frac{3{\rm e}14}{g}\right) \rho^{1/3} \ {\rm cm}$$

— Infinite 3D elongated Coulomb crystals develop unstable phonon modes, if the elongation exceeds a critical value, <10% for most stretch directions (DB & Kozhberov 2017, DB & Chugunov 2018) Infinite 3D elongated Coulomb crystals develop unstable phonon modes, if the elongation exceeds a critical value, <10% for most stretch directions (DB & Kozhberov 2017, DB & Chugunov 2018)
Overstretched crystal layers will lose stability and get destructed as soon as their volume properties begin dominating

— Infinite 3D elongated Coulomb crystals develop unstable phonon modes, if the elongation exceeds a critical value, <10% for most stretch directions (DB & Kozhberov 2017, DB & Chugunov 2018)

— Overstretched crystal layers will lose stability and get destructed as soon as their volume properties begin dominating

— Since these layers have already cooled below melting, they can then freeze anew, somewhat above the destruction edge, into a stretch-free cubic structure

— Infinite 3D elongated Coulomb crystals develop unstable phonon modes, if the elongation exceeds a critical value, <10% for most stretch directions (DB & Kozhberov 2017, DB & Chugunov 2018)

— Overstretched crystal layers will lose stability and get destructed as soon as their volume properties begin dominating

— Since these layers have already cooled below melting, they can then freeze anew, somewhat above the destruction edge, into a stretch-free cubic structure

— Above this new cubic seed, the process of freezing with gradual stretching will repeat itself

To summarize, in contrast to the standard picture of cubic lattice formation, which is based on <u>energetics</u> argument but does not take into account <u>kinetics of growth</u>, neutron star crusts and white dwarf cores are made of elongated crystals. This has several astrophysical implications, the most obvious being for elastic properties of matter.

Part II: Applications

— Consider the strength of the stretched crystals with respect to shear deformations in planes orthogonal to the stretch

— Consider the strength of the stretched crystals with respect to shear deformations in planes orthogonal to the stretch

— This is relevant for NS and WD physics, where the stretch is aligned with the gravity, whereas the shear, caused for instance by magnetic field evolution, is horizontal and does not perturb hydrostatic equilibrium

— Consider the strength of the stretched crystals with respect to shear deformations in planes orthogonal to the stretch

— This is relevant for NS and WD physics, where the stretch is aligned with the gravity, whereas the shear, caused for instance by magnetic field evolution, is horizontal and does not perturb hydrostatic equilibrium — To find breaking strain, we looked for unstable phonon modes [i.e. modes with imaginary frequencies (DB & Kozhberov 2017)] for crystals, that were stretched by a factor ξ and then sheared in the perpendicular plane



$$u_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial r_j} + \frac{\partial u_j}{\partial r_i} \right)$$
$$u_{\theta\eta} = u_{\eta\theta} \equiv \frac{\varepsilon}{2} = \frac{\theta}{2\eta}$$

— Striking differences in breaking strain behaviour vs. stretch orientation

— A very significant elongation is possible along the cube edge

— For stretches along the cube diagonal, the breaking strain drops abruptly for contractions but gradually for elongations

— For stretches along the face diagonal, the situation is exactly opposite



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

$$u_{\theta\eta} = u_{\eta\theta} \equiv \frac{\varepsilon}{2} = \frac{\theta}{2\eta}$$

— It is not known what is the proper way of deducing crust properties from those of perfect crystallites

— Different stars may have different crust microstructure

— A plausible model may be to assume that, in a horizontal layer, there are crystallites <u>stretched</u> <u>vertically by approximately the</u> <u>same factor ξ but oriented more or</u> <u>less randomly</u>



Experiments on bicrystals, e.g. lead bicrystal from Rosenberg and Tiller (1957) show that crystals with different liquid-solid interface orientations can grow side by side



$$u_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial r_j} + \frac{\partial u_j}{\partial r_i} \right)$$
$$u_{\theta\eta} = u_{\eta\theta} \equiv \frac{\varepsilon}{2} = \frac{\theta}{2\eta}$$

2

— Under a shearing deformation, the crystallites will have the same strain to maintain continuity, and the crystallite with the minimum breaking strain will fail first. This may result in a stability loss and failure of neighbouring crystallites

$$\varepsilon_{\text{crit}} = 0.0639 - 20.1 (\xi^{2/3} - 0.99625)^2 - 2.33e6 (\xi^{2/3} - 1.00145)^6$$



— Effective shear modulus $\mu_{\text{eff}}(\xi)$.

— To calculate it at arbitrary ξ , apply an infinitesimal shearing deformation to a crystal stretched in a particular direction then evaluate the energy difference δU

$$\frac{\delta U}{V} = 2\mu u_{\theta\eta}^2$$

- Average μ over the shearing deformation azimuthal angle - Reproduced Fuchs's results for S_{1212} for bcc (0.1827) and fcc (0.1852) - Average over 7 stretch orientations, since strain in all crystallites is same. - $\mu_{eff}(1)=0.116$ or 0.114 depending on details of averaging ($\mu_{eff}^{OI}=0.1194 n_i U_C$) — LPE is a near-equilibrium process, which produces crystal layers of extremely high quality

— Is it possible that <u>near-equilibrium freezing with extremely uniform</u> <u>temperature and composition distributions and plenty of anneal time</u> in NS crusts and especially in WD cores produces large-scale near perfect crystallites?

— On Earth, natural <u>single</u> crystals as large as ~ 18 m (and possibly ~ 50 m) have been found (Rickwood, 1981)

American Mineralogist, Volume 66, pages 885-907, 1981

The largest crystals

PETER C. RICKWOOD

School of Applied Geology University of New South Wales Kensington, N.S.W. 2033, Australia

Abstract

No upper limit on the size of crystals is to be expected, but the dimensions a of the largest known crystals in each of twenty-four categories (nine classes)

— The occurrence of so huge natural crystals indicates, at least, that there are robust mechanisms of seeding their growth — In an experiment of Rosenberg & Tiller (1957) purified lead was melted and poured into a mold designed for unidirectional (upward) freezing

— Subsequent analysis of the ingot had shown that there were <u>no</u> <u>crystallites other than those, which nucleated on the bottom boundary</u>

— The ingot bottom surface had 10 times as many crystallites as the top one

— This means that <u>90% of the original crystallites have been crowded out</u> by the surviving ones

— The preferred orientation of crystallite growth was close to perpendicular to $\{111\}$ planes

— However, the conditions of these experiments were far from equilibrium



— Also of interest are Czochralski, Stockbarger, and other crystal growth techniques in semiconductor industry, which produce 1-2 m long <u>ideal</u> crystals

— These processes are subject to severe limitations posed by <u>finite sizes of</u> <u>the apparatus and associated with them nonuniformities, thermal gradients</u> <u>and stresses</u>



— According to Bravais's rule, in equilibrium, crystals tend to grow towards a <u>shape bounded by the slowest growing planes</u>

- The fastest growing surfaces grow themselves out
- <u>The slowest growing planes are the close-packed ones</u>
- These are $\{110\}$ planes for bcc crystals and $\{111\}$ planes for fcc
- The rule is supported by prominence of {111} plane growth in various experiments on Earth predominantly conducted on fcc materials

Should we then expect that the entire crystallization front in a compact star grows perpendicular to {110} planes of <u>stretched bcc</u> lattices or perpendicular to {111} planes of <u>stretched fcc</u> lattices?
This is a distinct possibility!

— This may lead to astrophysical manifestations of properties of specific crystallites rather than of average (or minimum) properties

$$\frac{n_{\rm e}}{\nabla n_{\rm e}} = \frac{4}{3}h_P = \frac{4P_{\rm e}}{3\rho g} = \frac{4}{3}\left(\frac{3Z}{A}\right)^{4/3}\left(\frac{3{\rm e}14}{g}\right)\,\rho^{1/3} \ {\rm cm}$$

— For {111} growth, at density 10^9 g/cc, it takes ~2 m to grow to a critical height

— Do not expect ~10 m tall crystallites in the outer layers of NS (Caplan+2018), but lateral sizes of this magnitude <u>or more</u> do not seem impossible

— The descending portion of the $\varepsilon_{crit}(\xi)$ curve is approximately linear from $\xi=1$ to ξ_{max} . This indicates the presence, upon freezing, of layers with breaking strain for shear <u>much lower than at $\xi=1$ </u>

— Specifically, there is a layer of ~ 20 cm thick, in which the breaking strain is 10 times lower, and a layer of ~ 2 cm thick, in which the breaking strain is 100 times lower, than for the bulk of the crystallite

— If, under the action of magnetic or any other stresses late in a NS evolution, these layers break and then refreeze into a stress-free cubic configuration, they become 10 or 100 times stronger and do not break that easily at a later time

— The diversity of layer sizes and strengths as well as the possibility of significant strengthening of matter after breaking and refreezing may help explain rich magnetar burst and outburst phenomenology and its extension to lower-B objects

— Stretched crystals have higher ground-state energy, than the cubic ones (DB & Chugunov, 2018), and the difference, in principle, may be released. This may occur at arbitrarily late cooling stages. For WD, this may happen at an age, when the stellar luminosity is already very low, and thus it <u>may</u> noticeably delay WD cooling

