Multinary compounds in neutron-star crusts

N. Chamel[1], A. F. Fantina[1,2]

[1]Institut d'Astronomie et d'Astrophysique, CP-226, Université Libre de Bruxelles, 1050 Brussels, Belgium

[2]Grand Accélérateur National d'Ions Lourds, CEA/DRF - CNRS/IN2P3, Bvd H. Becquerel, 14076 Caen, France

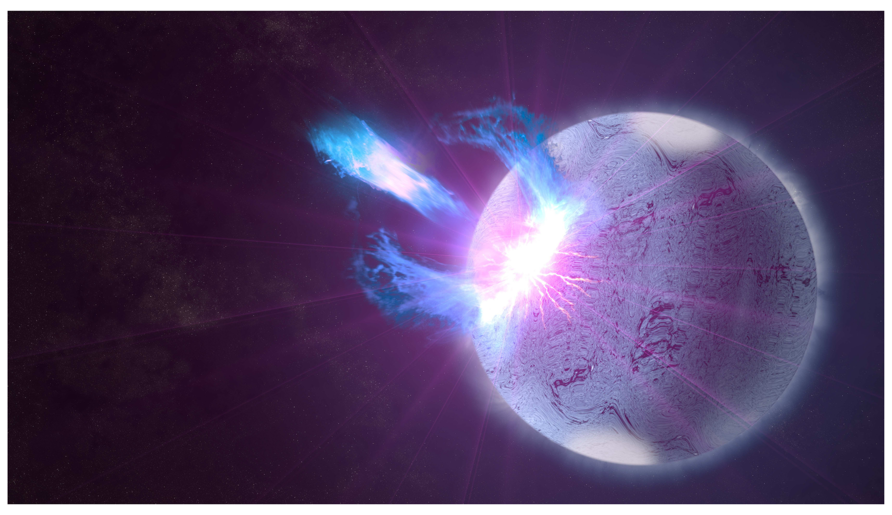
Abstract

The outer crust of a neutron star has been generally assumed to be stratified into different layers, each of which consists of a pure body-centred cubic ionic crystal in a charge compensating electron background. The validity of this assumption is examined by analysing the stability of multinary ionic compounds in dense stellar environments. It is shown that their stability against phase separation is uniquely determined by their structure and their composition irrespective of the stellar conditions. However, equilibrium with respect to weak and strong nuclear processes imposes very stringent constraints on the composition of multinary compounds, and thereby on their formation. By examining different cubic and noncubic lattices, it is found that substitutional compounds having the same structure as cesium chloride are the most likely to exist in the outer crust of a nonaccreting neutron star.

I Introduction

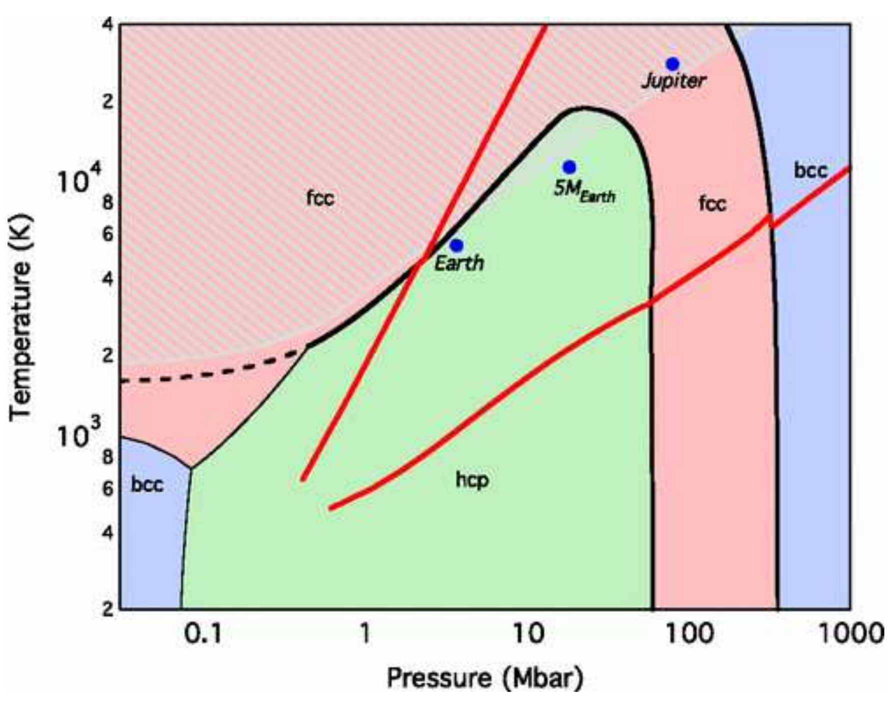
Many properties of the crust of a neutron star are determined by its structure, which in turn have implications for various astrophysical phenomena:

- (small) Crab like pulsar sudden spin-ups,
- thermal relaxation in transiently accreting stars,
- giant flares from soft gamma-ray repeaters and quasiperiodic oscillations,
- gravitational wave emission (mountains).



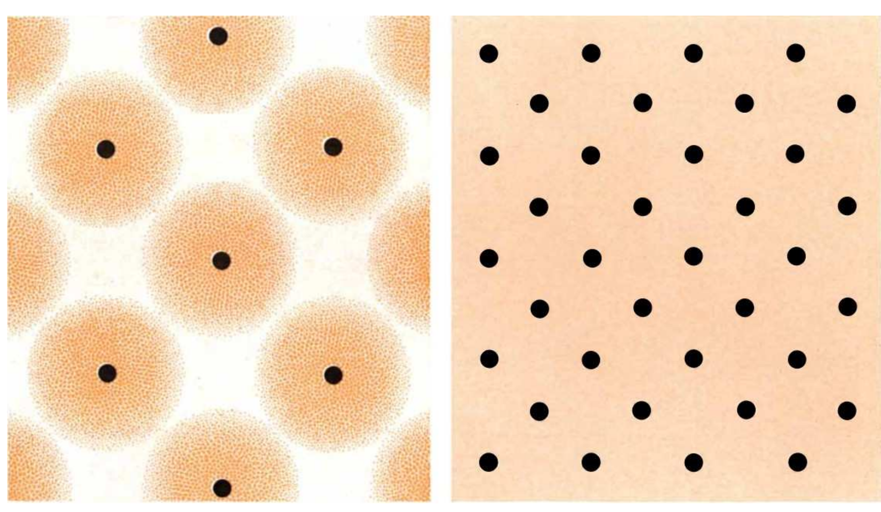
Artistic view of a magnetar "storm". Credit: NASA's Goddard Space Flight Center/S. Wiessinger.

The outermost region of a nonaccreting neutron star is expected to be made of iron ^{56}Fe, the end-product of stellar nucleosynthesis. The properties of compressed iron can be probed in terrestrial laboratories up to pressures of order 10^{14} dyn cm^{-2} with nuclear explosions and laser-driven shock-wave experiments. Under these conditions, iron has an hexagonal close-packed structure [1]. Ab initio calculations predict various **structural phase transitions** at higher pressures.



Phase diagram of compressed iron. Figure taken from Ref. [1].

Although such pressures are tremendous according to terrestrial standards, they still remain negligibly small compared to those prevailing in a neutron star. Deeper in the star, at a density $\rho_{\rm eip} \approx 2\times 10^4$ g cm^{-3}, the interatomic spacing becomes comparable with the atomic radius. At densities $\rho \gg \rho_{\rm eip}$, atoms are crushed into a **dense plasma of nuclei and free electrons**. Beyond this point, electrons are very weakly perturbed by ions, and thus behave as an essentially ideal Fermi gas.

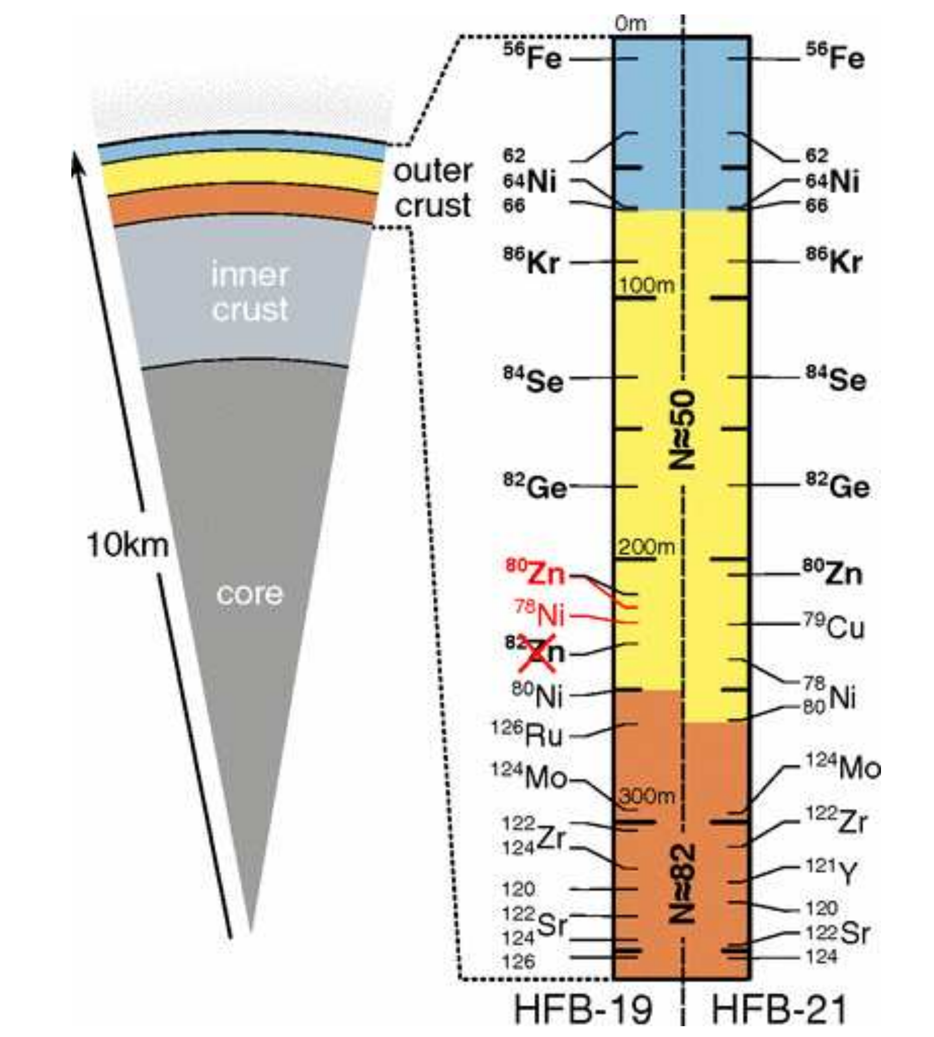


Distribution of electrons in a terrestrial solid (left) and in the crust of a neutron star (right). Figure taken from Ref. [2].

It has been generally assumed that nuclei are arranged in a **body-centered cubic** (bcc) lattice, as put forward by Ruderman [3] based on the pioneer cubic-lattice constant calculations of Klaus Fuchs [4]. However, in the presence of different nuclear species, other solid structures may form. We have thus recently studied the existence of **multinary ionic compounds** [5].

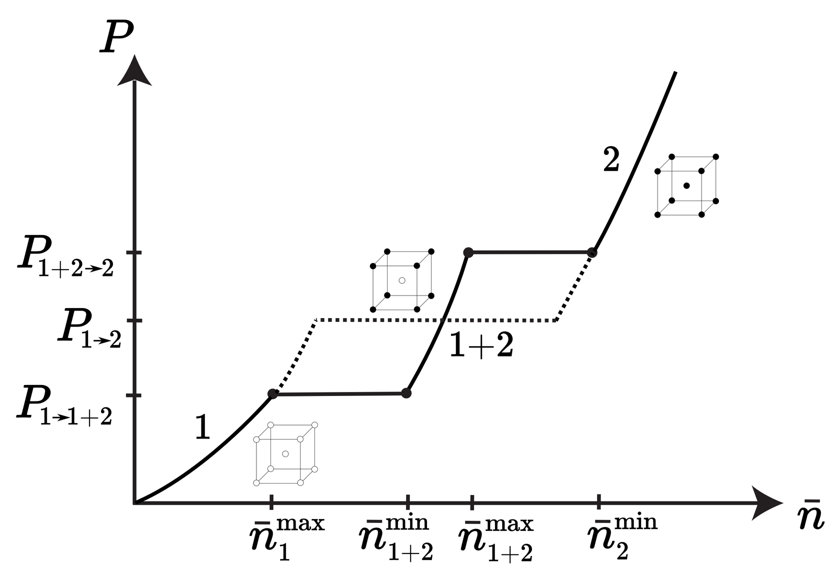
II Formation of multinary compounds

The outer crust of a neutron star is usually thought to consist of pure bcc layers made of only of type of nuclei (see, e.g. Ref. [6]).



Composition of the outer crust of a nonaccreting neutron star, as predicted by two different nuclear mass models. The presence of ^{82}Zn predicted by HFB-19 was ruled out by experiments at the ISOLDE-CERN facility. Figure taken from Ref. [7].

In principle, pure bcc phases could coexist. However, such **mixed solid phases cannot be present in a neutron star crust** because the pressure has to increase strictly monotonically with density.



Schematic representation of the pressure P versus mean baryon number density $\bar{n}$ for a transition between two pure solid phases accompanied by the formation of a binary compound. The phase coexistence is indicated by dotted lines. Figure taken from Ref. [5].

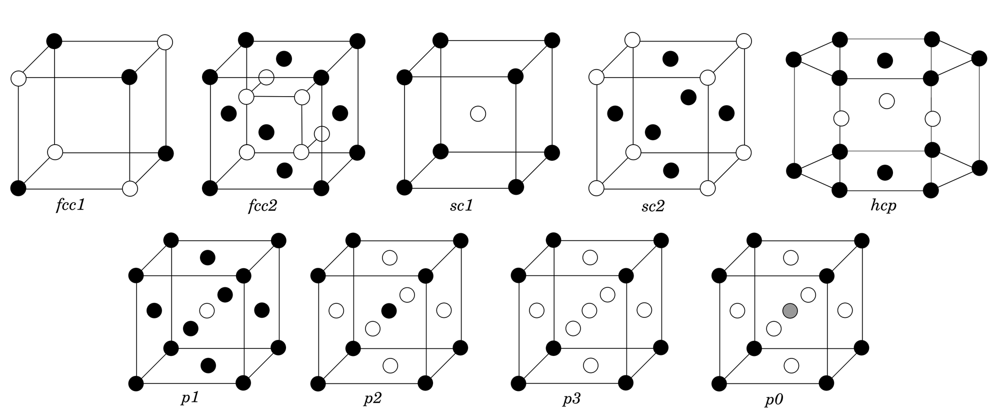
In 1971, Dyson [8] suggested the existence of FeHe compound with rocksalt structure. This possibility was further studied by Witten in 1974 [9]. However, as pointed out by Jog&Smith [10], such a compound is unstable against weak and strong nuclear processes. On the other hand, they found that binary compounds with cesium chloride structure can be energetically favored at the interface between two crustal layers. Because ion charges are similar, disordered compounds are unstable and will not be further considered [11].

A multinary compound made of nuclei with charges $\{Z_i\}$ could exist in the crust of a neutron star if it is **stable against the separation into pure (bcc) phases** [5]:

$$\mathcal{R}(\{Z_i/Z_j\}) \equiv \frac{C}{C_{\rm bcc}} f(\{Z_i\}) \frac{\bar{Z}}{\overline{Z^{5/3}}} > 1 \qquad (1)$$

where $f(\{Z_i\})$ is the dimensionless lattice structure function of the compound and C the corresponding structure constant. For a pure crystal, $f(Z)=Z^{2/3}$. This shows that **the stability of a compound is independent of the stellar environment**, as recently noticed in Ref. [12] from a systematic search of equilibrium phases.

We have investigated the formation of various binary and ternary compounds:



Terrestrial examples:

- fcc1: rocksalt (NaCl), oxydes (MgO), carbonitrides (TiN)
- fcc2: fluorite (CaF_2)
- sc1: cesium chloride (CsCl), β-brass (CuZn)
- sc2: auricupride ($AuCu_3$),
- hcp: tungsten carbide (WC),
- p0: cubic perovskite ($BaTiO_3$).

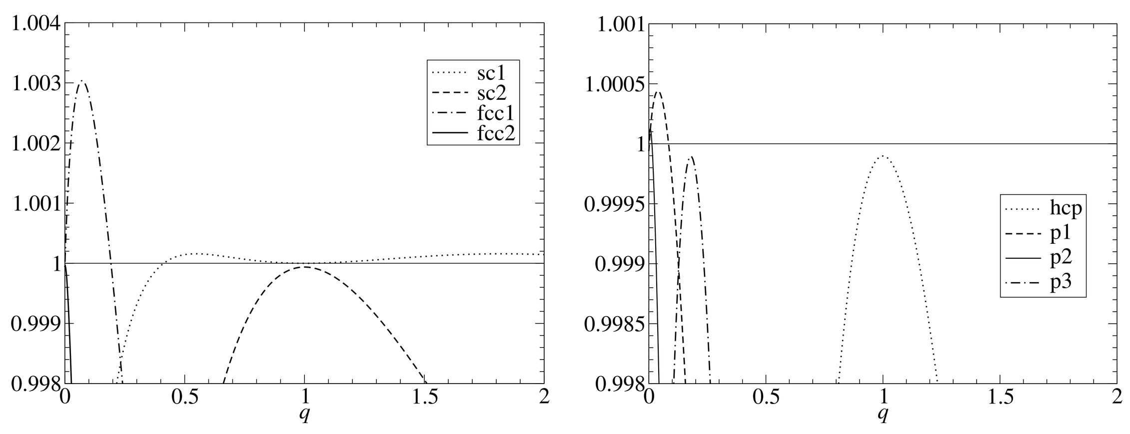
Stellar compounds differ in two fundamental ways from their terrestrial counterparts: (i) they are made of "bare" nuclei; (ii) electrons form an essentially uniform relativistic Fermi gas.

The structure functions of a binary compound can be generally written as

$$f(Z_1,Z_2) = \bar{Z}^{-4/3}\Big[\eta Z_1^2 + \zeta Z_2^2 + (1-\eta-\zeta)Z_1 Z_2\Big]\,, \qquad (2)$$

$$\mathcal{R}(Z_1,Z_2) = \mathcal{R}(q\equiv Z_2/Z_1)) = \frac{C}{C_{\rm bcc}} \frac{\eta + (1-\eta-\zeta)q + \zeta q^2}{\Big[\xi + (1-\xi)q\Big]^{1/3}\Big[\xi+(1-\xi)q^{5/3}\Big]}\,, \qquad (3)$$

where ξ denotes the proportion of nuclei (A_1,Z_1). Similarly, for a ternary compound $\mathcal{R}$ depends on the charge ratios only. **Compounds with sc2, fcc2, p3 and hcp structures are unstable against phase separation for any charge ratio since $\mathcal{R}<1$** [5]:



The sc1, fcc1, p0, p1, and p2 structures can lead to stable compounds depending on the charge ratios. In particular, the fcc1 structure with a charge ratio $q \simeq 0.07$ yields the most stable compounds with $\mathcal{R}\simeq 1.003$, as first pointed out by Dyson [8]. However, such compounds are not necessarily stable against weak and strong nuclear reactions. Compounds with the sc1 structure are the most likely to be present in the neutron-star crust since they are stable over a very wide range of charge ratios, from $q\simeq 0.413$ to $q\simeq 2.42$. This conclusion is consistent with Monte Carlo simulations [13].

Using experimental atomic mass data from the 2012 AME [14] supplemented with the microscopic HFB-24 nuclear mass model [15], we have calculated the ground-state structure and the equation of state of the outer crust of a cold nonaccreting neutron star allowing for compounds. These calculations have confirmed that **binary compounds with sc1 structure can form at the boundary between pure crustal layers**. We have also obtained very accurate analytical formulas for the threshold pressure and the densities of the solid phases. We have thus shown that **stellar compounds made of different isotopes are unstable**.

V Conclusions

The stability of a multinary compound against phase separation is shown to be uniquely determined by its structure and its composition irrespective of the stellar conditions, and can thus be easily tested through the criterion (1).

Equilibrium with respect to weak and strong nuclear processes imposes stringent constraints on the composition of neutron-star crusts. Full numerical results can be found in Ref. [5], as well as very accurate analytical expressions. We have shown that only substitutional compounds with cesium chloride structure can form at the interface between two pure layers. Their presence may have important implications for the thermal and mechanical properties of the crust [16, 17, 18]. In our study, we have neglected electron exchange and polarization effects, as well as quantum zero point motion of ions. The influence of these corrections needs to be examined.

From our analysis, we expect a much large variety of ordered and disordered multinary compounds to form in the crust of accreting neutron stars.

This work was mainly financially supported by FNRS (Belgium). Partial support comes also from the COST Action MP1304. The authors thank D. G. Yakovlev and A. A. Kozhberov for valuable discussions.

References

[1] L. Stixrude, Phys. Rev. Lett. **108**, 055505 (2012).
[2] M. Ruderman, Scientific American **224**, 24 (1971).
[3] M. Ruderman, Nature **218**, 1128 (1968)
[4] K. Fuchs, Proc. B. Soc. London A **151**, 585 (1935).
[5] N. Chamel, A. F. Fantina, Phys. Rev. C **94**, 065802 (2016).
[6] J. M. Pearson, S. Goriely, and N. Chamel, Phys. Rev. C **83**, 065810 (2011).
[7] R. N. Wolf et al., Phys. Rev. Lett. **110**, 041101 (2013).
[8] F. J. Dyson, Ann. Phys. **63**, 1 (1971).
[9] T. A. Witten, Astrophys. J. **188**, 615 (1974).
[10] C. J. Jog and R. A. Smith, Astrophys. J.**253**, 839 (1982).
[11] T. Igarashi, N. Nakao, H. Iyetomi, Contrib. Plasma Phys. **41**, 319 (2001).
[12] T. A. Engstrom, N. C. Yoder, V. H. Crespi, Astrophys. J. **818**, 183 (2016).
[13] S. Ogata, H. Iyetomi, S. Ichimaru, Phys. Rev. E **48**, 1344 (1993).
[14] G. Audi, M. Wang, A. H. Wapstra, F. G. Kondev, M. MacCormick, X. Xu, B. Pfeiffer, Chin. Phys. C **36**, 1287 (2012).
[15] S. Goriely, N. Chamel, J. M. Pearson, Phys. Rev. C **88**, 024308 (2013).
[16] A. A. Kozhberov and D. A. Baiko, Contrib. Plasma Phys. **52**, 153 (2012).
[17] A. A. Kozhberov and D. A. Baiko, Physics of Plasmas **22**, 092903 (2015).
[18] T. Igarashi, H. Iyetomi, J. Phys. A**36**, 6197 (2003).