Title: The Breaking Strain of Neutron Star Crust

Author(s): Kai Kadau, T-1
C. J. Horowitz, Indiana University

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Mountains on rapidly rotating neutron stars efficiently radiate gravitational waves. The maximum possible size of these mountains depends on the breaking strain of neutron star crust. With multi-million ion molecular dynamics simulations of Coulomb solids representing the crust, we show that the breaking strain of pure single crystals is very large and that impurities, defects, and grain boundaries only modestly reduce the breaking strain to around 0.1. Due to the collective behavior of the ions during failure found in our simulations, the neutron star crust is likely very strong and can support mountains large enough so that their gravitational wave radiation could limit the spin periods of some stars and might be detectable in large scale interferometers. Furthermore, our microscopic modeling of neutron star crust material can help analyze mechanisms relevant in Magnetar Giant and Micro Flares.

"Mountains" on rapidly rotating neutron stars (NS) can efficiently radiate gravitational waves (GW) because of their large masses and high accelerations [1]. Searches for these waves are presently underway with large scale interferometers [2]. Furthermore, the angular momentum radiated could control the spin periods of some accreting NS [3]. As material falls on a NS, from its binary companion, the angular momentum accreted spins up the star. However, GW radiation increases very rapidly with rotational frequency. The star may reach spin equilibrium where the angular momentum gained from accretion is balanced by GW radiation. This could explain why the most rapidly spinning pulsars observed are only spinning at about half of the breakup rate.

How high can a mountain be, before it collapses under the NS's extreme gravity? This depends on the breaking strain (BS) [23] of NS crust (NSC) which is the fractional deformation when the crust fails. Estimates of the BS vary by orders of magnitude and are based on lose analogies with conventional materials rather than on detailed calculations or simulations [4]. This is, perhaps, the largest uncertainty for predictions of these GW. In this paper we use molecular dynamics (MD) simulations to significantly improve estimates of the BS.

Crust breaking may also be important for Magnetar Giant Flares. These are extremely energetic Gamma-ray bursts from strongly magnetized NS [5]. Thompson and Duncan model Giant Flares as "star quakes" [6]. A strong twisted magnetic field stresses the crust until it breaks. The crust then moves and allows magnetic field lines to reconnect. This releases magnetic energy that powers the flare. Although the bulk of the flare's energy comes from the magnetic field, rather than the elastic energy stored in the crust, this mechanism may still require the crust to be relatively strong in order for it to control the very strong magnetic field.

How the crust breaks may be important for the excitation of NS oscillation modes from a "star quake". Quasiperiodic oscillations have been observed in the tails of Giant Flares [7, 8]. These have been interpreted as shear oscillations of the NSC. If these modes can be convincingly identified, they may provide considerable information on the structure of the NS and its crust [9]. In addition, LIGO (Laser Interferometer Gravitational Wave Observatory (CalTech/MIT)) has searched for GW from a Magnetar Giant Flare that could come from large amplitude NS oscillations [10]. Our simulations of crust breaking may lead to insight into the excitation of these modes and the amplitudes that might be expected.

In addition to the very rare Giant Flares, Magnetars also emit less energetic, but more common, flares and micro-flares [11]. Perhaps these are related to crust cracking, rather than breaking. Here, the presented simulations could provide insight into the mysterious relation between flares and Giant Flares.

In the crust of a NS, electrons form a very degenerate relativistic gas. The ions are completely pressure ionized and have Coulomb interactions that are screened at large distances by the slightly polarizable electron gas. The interaction between two ions $i,j$ is assumed to be a screened Coulomb or Yukawa potential [12],

$$\phi(r_{ij}) = \frac{Z^2 e^2}{r_{ij}} e^{-r_{ij}/\lambda},$$  \hspace{1cm} (1)

where the ions have charge $Z$, $r_{ij}$ is the distance be-
between them, and the electron screening length \( \lambda_e = \pi^{1/2}/2e(3\pi^2n_e)^{1/3} \) with \( n_e \) the electron density. The total potential energy is given by the sum over all pairs \( \sum_{i<j} \phi(r_{ij}) \). Charge neutrality insures that \( n_e = Zn \) where \( n \) is the ion density. The ions are assumed to form a classical one component plasma that can be characterized by the Coulomb parameter \( \Gamma \),

\[
\Gamma = \frac{Z^2 e^2}{\varepsilon_0 a T}.
\]  

(2)

This is the ratio of a typical Coulomb energy to thermal energy and the ion sphere radius \( a = [3/(4\pi n)]^{1/3} \) is a typical distance between ions.

We calculate at a reference density of \( n = 7.18 \times 10^{-5} \text{ fm}^{-3} \) using \( Z = 29.4 \) and an atomic mass number \( A = 88 \) \( (1 \times 10^{13} \text{ g/cm}^3) \) [13]. Results can be scaled to other densities at constant \( \Gamma \) and approximately scaled to other \( Z \) at constant \( \Gamma \), which involves only a small change in \( \lambda_e \). Most of our simulations are for a temperature \( T = 0.1 \text{ MeV} \). This corresponds to \( \Gamma = 834 \). We ignore the effects of free neutrons that are present in the inner crust.

We perform large-scale MD simulations of shearing NSC material as we believe that this is the most important mode of failure in the crust. Tension simulations at constant volume, had a breaking strain and strength that was smaller by 2.5 and 2, respectively. We use two independent MD codes: YukawaMD is a serial MD code where the system is strained by moving a boundary layer of frozen ions on top and bottom against each other [15],[25] We cutoff the potential at the large distance \( r_{\text{cut}} = 10\lambda_e \) resulting in each ion interacting with about 5400 neighbors; for smaller values of \( r_{\text{cut}} \) the results depend on \( r_{\text{cut}} \) [16] (Figs. S1 and S2). [26]

Figure 1 shows the shear stress versus strain for body-centered cubic (bcc) crystals as is the equilibrium structure at the given density and \( \Gamma \); some results for the face-centered cubic (fcc) structures are added as some metastable fcc phase might be present in the crust as well. For all investigated crystallographic shear systems the perfect crystals all show a BS well above 0,1, and break in a rather abrupt fashion with only a very small region where plasticity, i.e. deviation from a linear stress-strain relation, is present. The multi-million ion systems were strained at a rate of \( 4 \times 10^{-7} \text{ c/fm} \). As we cannot simulate the very large time and length scales associated with NSC we have to rely on estimates based on a series of simulations that suggested basically no size effects for the single crystal simulations presented here (Fig. S3) and a converging result at low shear rates (Fig. S4). We also note that tripling the temperature only reduces the maximum stress by about 25% and does not significantly alter the BS.

As very little is known about the defect structure, grain sizes, and associated grain boundaries of NSC that potentially can reduce the strength, we also consider polycrystalline materials that are generated using a Voronoi construction in which grain centers and orientations are picked at random and each ion belongs to the grain center that is closest [17]. After this initialization, the system is equilibrated by heating it from 0.1 to 0.3 MeV and back to 0.1 MeV over a total simulation time of 275000 fm/c. The system is then sheared at a strain rate of \( 4 \times 10^{-7} \text{ c/fm} \). Figure 2 shows one system with 12.8 million ions at strains of 0.0, 0.05, 0.1, and 0.15 (for stress-strain curve see Fig.1). The radial distribution functions exhibit characteristic peaks of the bcc structure for strains up to 0.1. After failure, at 0.15 strain some degree of amorphization might be possible. The system starts to deform plastically near the grain boundaries in a collective manner without exhibiting signs of dislocations or other more localized events (Fig.2 and movie S5). However, at large strains the samples are plastically deformed and the mode of failure seems to be a reorientation of local regions —possibly associated with some degree of amorphization (Fig.2) — to accommodate the shear. This collective, rather than more localized dislocation-based, mode of plasticity makes the crystal stronger and break at larger strains than terrestrial metals, where the electronic density can have a localized structure to accommodate local defects. This failure mechanism also does not allow for voids or fracture to appear as these localized defects would possibly heal under the influence of the high pressure. In fact, simulations that started out with a cylindrical hole with a diameter of 2.5x the nearest neighbor distance initialized into the otherwise perfect.
FIG. 2: Polycrystalline sample with 12.8 million ions consisting of 8 differently oriented grains with an average grain diameter of 3961 fm at strains of 0.0, 0.05, 0.1, and 0.15. Upper panel: The radial distribution functions at different shear states exhibit the characteristic peaks of the bcc structure for strains up to 0.1. At 0.15 strain some degree of amorphization might be possible. Lower panel: At 0.0 strain the eight different grains are shown in different colors. At strains of 0.05, 0.1, and 0.15 the red color indicates plastic deformation, i.e. distortions of the ions away from an ideally uniformly sheared bcc lattice in the range of 0 to two times the nearest neighbor distance. Note that the top and bottom layers are frozen and moved to impose the shear.

We investigated samples with grain diameters between 570 fm and 3961 fm that showed a clear monotonic trend to increase the BS and stress with the grain size. As we expect to have larger grains in NSC material than we could possibly simulate on a computer we expect the crust material strength only to be slightly reduced by the presence of grain boundaries. Also, note that accreting NS can form new crust very slowly over accretion times of thousands of years. This should allow plenty of time for larger crystals to form. Second, samples with very small grain size may have a reduced thermal conductivity and this could disagree with crust cooling observations [20, 21]. Indeed, the grain size could be much larger than in our simulations. In that case, we expect the strength of the system to be larger and closer to our single crystal results.

To study the role of impurities we form a 27648 ion crystal made of the complex rapid proton capture nucleosynthesis ash considered in ref. [13]. We use the solid composition from Table I of ref. [13]. This includes a range of ions from $Z = 8$ to 47 and can be characterized by an impurity parameter $Q = (Z^2) - (Z) = 22.3$ that describes the dispersion in ion charges. Sheternin et al. [21] and Cumming and Brown [20] study the rapid crust cooling of two NS, after extended outbursts. Cumming and Brown conclude that $Q$ must be less than 10 [20], see also [19]. Otherwise impurities would reduce the crust thermal conductivity by too much to agree with observation. Our crystal has more impurities than this limit. Therefore, we believe our results may represent an upper limit on the effects of impurities. Indeed, we have so many impurities that our runs with significantly more impurities phase separate [13]. We equilibrate our crystal by heating it up and then slowly cooling it back down to $T = 0.1$ MeV over a total simulation time of about 85 million fm/c. We shear this crystal at a strain rate of $8 \times 10^{-7}$ c/fm and find a maximum stress that is reduced from the maximum stress of a pure crystal by less than 45% at a similar strain. We conclude that impurities are unlikely to significantly reduce the strength of NSC.

Our simulations show that the breaking strength of NSC—the strongest material known—is about $10^{10}$ times more than for terrestrial engineering materials such as metal-alloys where the strength is measured in fractions of a GPa. The largest contributor to this tremendous difference is of course the enormous pressure and thus density in NSC. Furthermore, the screened Coulomb interaction is purely repulsive and has no explicit length scale [27], i.e. the system at twice the density behaves just like the system at the original density only at a lower temperature (Eq. 2). This causes the material to fail abruptly in a collective manner at a large strain, rather than yielding continuously at low strain as observed in metals, because of the formation of dislocations. This different response of Coulomb solids to deformations could provide insight into designing improved materials. Note that small Coulomb solids have been studied in the laboratory using cold trapped ions [22].
In conclusion, we have performed large-scale MD simulations of the breaking strain (BS) of Coulomb solids representing neutron star crust (NSC). We find a collective mode of failure that does not involve localized defects such as dislocations, opening of voids, or fractures. The BS in the presence of introduced defects and impurities is only moderately reduced to about 0.1. The large BS, that we find, should support mountains on rapidly rotating NS large enough to efficiently radiate gravitational waves. This may motivate further work on mountain forming mechanisms and searches for continuous gravitational waves. Furthermore, the methods we presented here are very promising to describe other aspects of Coulomb solids and NSC in particular.

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Fig. S1 (screened-coulomb.ps)
The screened Coulomb potential (Yukawa potential) with no cut-off (red line) as compared to various cut-offs and cut-off boundary conditions. The derivative of the potential at the cut-off can be forced to be zero by multiplying the potential with \((1-(r/r_c)^10)^2\).

Fig. S2 (stress-strain-cut.ps)
Shear stress dependence of the cut off distance at a rate of $4 \times 10^{-7}$-c/fm as calculated with the SPaSM code. The YukawaMD code found a similar behavior for the cut off dependence.

Fig. S3 (stress-strain-size.ps)
Shear stress dependence of the system size at a rate of $4 \times 10^{-7}$-c/fm as calculated with the SPaSM code. Due to the different boundary conditions that impose the shear in the YukawaMD (deforming the periodic box) and SPaSM code (moving top and bottom frozen layer) the size dependence converges for smaller systems for the YukawaMD (around 5000 atoms) than for the SPaSM code.

Fig. S4 (stress_rate.pdf)
Shear stress, in units of $Z^2e^2n/a$, versus shear strain for a 9826 ion system as simulated with YukawaMD at strain rates of (left to right) 0.125, 0.25, 0.5, 1, 2, 4, 8, 16, and 32 $\times 10^{-8}$-c/fm.

Movie S5 (Neutron-crust-poly-8-grains-12.8million-part-0.1MeV-2NNdist.mov)
Polycrystalline sample with 12.8 million atoms consisting of 8 differently oriented grains with an average grain diameter of 3961 fm. The red color indicates plastic deformation, i.e. distortions of the ions away from an ideally uniformly sheared bcc lattice in the range of 0 to two times the nearest neighbor distance. Note that the top and bottom layers are frozen and moved to impose the shear after the initial relaxation process. The shear strain increases from 0 to about 0.16.
Screened Coulomb potential

no cut-off

\( r_c = 4\lambda, \phi(r_c) = 0, \phi'(r_c) = 0 \)

\( r_c = 5\lambda, \phi(r_c) = 0, \phi'(r_c) = 0 \)

\( r_c = 6\lambda, \phi(r_c) = 0, \phi'(r_c) = 0 \)

\( r_c = 8\lambda, \phi(r_c) = 0, \phi'(r_c) < 0 \)

\( r_c = 10\lambda, \phi(r_c) = 0, \phi'(r_c) = 0 \)

\( r_c = 12\lambda, \phi(r_c) = 0, \phi'(r_c) = 0 \)

Fig S1

screened_Coulomb.pdf
Movie S5

Neutron-crest-poly-grows