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The limits of strength in materials in the condensed phase

N K Bourne

Centre for Matter under Extreme Conditions, University of Manchester, Research Complex at Harwell, Rutherford Appleton Laboratory, Didcot, Oxfordshire, OX11 0FA, UK. Formerly at AWE, Aldermaston, Reading, RG7 4PR. United Kingdom.

E-mail: neil.bourne@manchester.ac.uk

Abstract. There is a range of thresholds in loading for the response of condensed phase matter, starting with inelastic deformation at the yield stress. Beyond this point compression continues until the material bond strength is overcome and becomes so-called warm dense matter. In this regime formulations of solid mechanics derived in the ambient state no longer apply. Between these two limits lies a boundary that differentiates weak- from strong-shock dynamic loading. This work examines these thresholds and shows a correlation between the theoretical strength of the material and this weak shock limit for a range of metals.

1. Introduction

The modern world requires understanding of behaviour in order to design materials and structures capable of surviving extreme mechanical loads [1]. One key requirement is the prediction of the strength of matter within those extreme environments and understanding of their limiting thresholds to define the zones in which they may operate. These might be quasi-static under conditions such as those pertaining to planetary cores or impulsive such as those found in satellite bombardment by extra-terrestrial or orbital debris [2, 3]. In either case the strength of solids is controlled by the energy needed to break a bond under mechanical load and these values are different in hydrodynamic compression and in static or dynamic shear. Further maximum shear strengths are particularly important for the generation and motion of defects under load. Thus the response is bounded by the maximum electronic bond strength permissible under these boundary conditions. A first step down this path is to predict affine deformation in perfect crystals under high compression. Here strength itself ceases to have an extended definition beyond the point at which the bonding is exceeded and new electronic conformations are established [4]. The theoretical compressive and shear strengths may be determined by a range of methods of increasing computational complexity using *ab initio* methods to determine values for particular slip systems in pure solids with either metallic or covalent bonding [5].

At greater scale within a general volume element, condensed matter may be regarded as a composite of crystals, granular boundaries with some degree of disorder, second phase particles, and included voids. As the loading amplitude increases, matter yields first at a defined yield stress with microstructure homogenizing as the loading level increases. Beyond the theoretical strength of material it simplifies to a regularly stacked conglomerate of crystalline and second phase regions alone [6]. Dynamic loading for short times or small sample sizes, leads to a small strain response in the lattice and such experimental observations may generally only be mapped to those obtained statically when temperature is directly comparable.

The super-extreme conditions for matter found in nature cover a range of thermo-mechanical states that are studied within high energy density physics [7]. A lower bound may be regarded as an energy density comparable to the valence electron binding energy of condensed matter (10^5 J cm^{-3}). The point at which bonding exceeds consideration of purely valence electrons (the *finis extremis* FE) occurs when the energy density of the impulse exceeds that of the outer bound electron, and beyond this value, strength (at least as understood in continuum mechanics in the ambient state) becomes an undefined quantity [8]. The FE threshold may be estimated at between *ca*. 100 and 300 GPa and varies for each element according to the electronic density of states in each element or compound considered. Beyond this threshold exists a further transition region where the electronic bonds between atoms become forced into new states localized in regions different to those observed under ambient conditions [4]. This un-ionized state is dubbed Warm Dense Matter (WDM).

An estimate of the highest stresses required to overcome the bond strength of materials can be recovered from calculation of their ultimate strength [5]. Rousseau and Ashcroft calculate the electron density for alkali metals at significant compression on a plane through the lattice [9]. They clearly show a localization of density through the lattice that approaches closer packing as compression proceeds. Beyond the FE threshold new electronic correlations are observed which relate directly to optical and insulator-metal transitions observed in metals. In this region the structures adopted by solids provide stringent tests of an ability to predict the forms and thermodynamic behaviour of high pressure states within condensed matter. Clearly concepts extrapolated from the yield surface used to extend solid mechanics become inapplicable since strength in the WDM region is ill defined [7]. Confirmation of the observed atomic structure comes primarily from diamond anvil data in this regime although diffraction observed using new techniques with a laser-driven shock impulse are providing information at the earliest times in the loading [10].

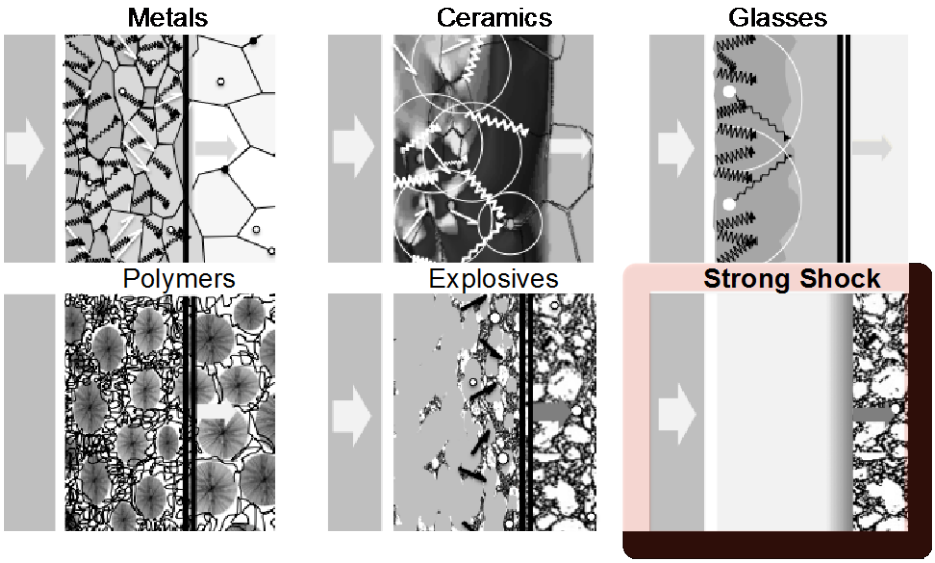

Figure 1. Schematic mesoscale weak shock response of a). metals, b). polycrystalline ceramics, c). glasses, d). thermoplastics, e). PBXs, f). loading in strong shock.

As matter is loaded to higher amplitudes the response of the material homogenises and variations in material characteristics become less prominent. The richest range of behaviours is found in the weak shock regime where defect structures dominate and their populations and geometry must be investigated and understood to explain response. The first phase of response will be densification at the largest pore volume in the microstructure. In all real materials there will be volume defects at some scale; from point defects at the microscale to pores at the meso- and component scales. If there is significant large scale porosity, as might be the case in foam or in a composite (glass microballoons are added to commercial explosives to sensitise formulations to shock for instance), then this must

close before plasticity at lower length scales can begin. A planar, spalled surface travels at twice the particle velocity behind the shock so that this defines an order of magnitude for a time of collapse. If the population has not closed before the impulse releases then later stages of compression cannot operate and the foam has absorbed the impulse.

Once the component has reached full density the three phases of response proceed sequentially as outlined above. Here the defect populations and the available flow mechanisms for metals, brittle solids, polymers and energetic materials determine the result in different material classes. Schematic responses for each class are shown in figure 1. Of course each individual material will have its own unique character either in composition, texture or defect population. However these straw men will serve as representatives of each to illustrate dynamic response. In each, a one-dimensional pulse at the continuum (component) scale is considered driven from left to right into a mesoscale composite. Localised flow surfaces are represented as zig-zag lines and porosity and grain boundaries are indicated in the microstructures. Of course in any real solid the impact surface has microstructure at the mesoscale on both the impactor or a target and this surface state will be important at lower scales representing a geometrical localisation zone which must be collapsed before flow may begin. However here it will be assumed that the surface state has the properties of the bulk and that the flow phase may commence instantaneously.

Snapshots of the response of metals and crystalline solids are shown in the top left of figure 1. The mesoscale structure consists of individual grains of particular stacked crystal phases, each with its own anisotropic structure and bonded with boundaries that have an intermediate disordered nature. There may be voids introduced within grains by processing or inclusions around which crystal growth has nucleated in the growth phase. At the microscale within the stacking there may be point defects or assemblages of lower density or merely regions where packing is disordered. Grain processing will mean that the crystals contain some population of line defects as well. All these features will result in a mesoscale texture which will determine initial ambient properties at the component scale.

The loading of the microstructure at the wavefront will start compression phases at different locations behind the front. The motion of atoms around defects will localise flow to weakened dislocation surfaces and compression can slip at these planes once they are established. The fastest processes in the crystal can proceed by a shuffle of atomic planes and this results in twinning or martensitic phase transformation within the crystals introducing a new boundary between phases of different stacking and accommodating a fixed proportion of strain within the target. Once localisation has settled the grain to a steady stress state, plastic flow may occur within it equilibrating the stress and strain states across the assembly of crystals within the mesoscale structure around. These processes occur by averaging the effect of each defect with wave propagation at that scale. Response of other classes of materials is also shown in the figure.

The lower left snapshot is a schematic of all classes of solid response in the strong shock regime. The front is strong enough to overcome the strength of the matter into which it progresses and deformation processes (and subsequent chemical reaction in the case of HE) are confined within that front. The flow behind it is homogeneous since all defects are activated so that no volume defects exist at the microscale excepting those that result from inhomogeneities of different elements. Further, the strains within shock fronts in typical experiments are always small so that mixing does not occur on microsecond time-scales. Thus the geometrical configuration of second phases is preserved when release arrives to cool the flow and re-establish a microstructure in the solid. In this state the material has density gradients and is at high temperature but response is homogeneous and whilst the shock front does not have a steady stress state, the flow behind has.

2. The Weak Shock Limit (WSL)

The definition of the weak shock limit is shown in figure 2. At the highest amplitudes, the shock is a step jump in pressure to the final state as a function of time or distance travelled through the target. Since solids have structure that must be overcome before the hydrodynamic state can be reached at lower stress levels, the picture is more complex. The Hugoniot now has an elastic and a plastic branch

(as shown to the left side of figure 2). The form of the curve is different since there are two loading regimes, elastic and plastic to consider. Both have different modes of behaviour which manifest themselves as alternate branches of the Hugoniot connected by a discontinuity at the Hugoniot Elastic Limit.

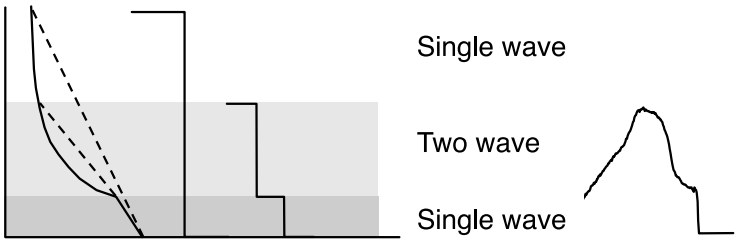

Figure 2. The weak shock limit (WSL). The evolution of Lagrangian stress profiles in elasto-plastic solids after shock loading. The critical value for pressure and wavespeed at the WSL is shown in red.

The transition from two-wave to single-wave shock structure represents a shift in regimes of behaviour. The stress range where two-wave structure exists is conventionally called the *weak shock* regime; that where it is overdriven, the *strong shock* regime. Typically the transition stress is at around ten times the Hugoniot elastic limit of the material but this value varies from solid to solid. It represents the point at which the defect density is saturated as discussed below and in what follows the transition stress/pressure will be dubbed the weak shock limit (WSL) P_{WSL}. To the far right of the figure is a real stress history from impact on a steel in the weak shock regime.

3. Results

The theoretical shear strength for the material may be computed using the Frenkel formulation and the relation between the pressure at the weak shock limit and the theoretical strength for a range of close packed metals is shown in figure 3 [5, 11]. The figure shows a faithful correlation between the theoretical strength and one third of the pressure in the deformed region. Each point in the figure represents a different element and two, tantalum and molybdenum, have been shown with the most sophisticated model generalized pseudopotential theory (MGPT) calculations for the strength [12]. There is an isotropic state beyond this stress, consistent with the removal of defects and a region within which interatomic repulsion alone controls the observed compression. To date the value of the theoretical shear strengths obtained experimentally most often come from the recalculated results of tensile tests for whiskers and is generally dominated by surface defects in the materials [5] but this offers a hitherto unexplored method of accessing this threshold using dynamic platforms. The derived pressure for the shock stress uses conservation of mass and momentum conditions with the closer equation that

$$U_{\mathrm{s}}=c_0+S\,u_{\mathrm{p}}=c_{\mathrm{L}} \tag{1}$$

Interestingly the state of dynamic compression that exists after the shock rise is at temperature whereas this is not so for quasi-static compression [13]. Clearly results of *ab initio* calculations are generally obtained for the absolute temperature equal to zero and correction of temperature due to phonons in the deformation processes approaches a one to one correlation with the data [14]. Nevertheless this result indicates that this threshold is not temperature sensitive and clearly not defect dependent as other determinations have always been in experiment. The rise time of the inelastic front itself is then that required for a kinetic temperature to equilibrate across the volume swept and below

the WSL this corresponds to the time taken for diffusion within the microstructure of a representative volume element (RVE) since this volume is inhomogeneous and localized hot spots exist until the peak of the wave. Once means of moving to denser packing is via strain-induced, displacive transformations which are observed to occur below the WSL in the solids enumerated here. Despite the simplicity of the Frenkel model, it should be noted that this is close to *ab initio* calculated values indicating the fundamental nature of this transition stress in condensed phase materials.

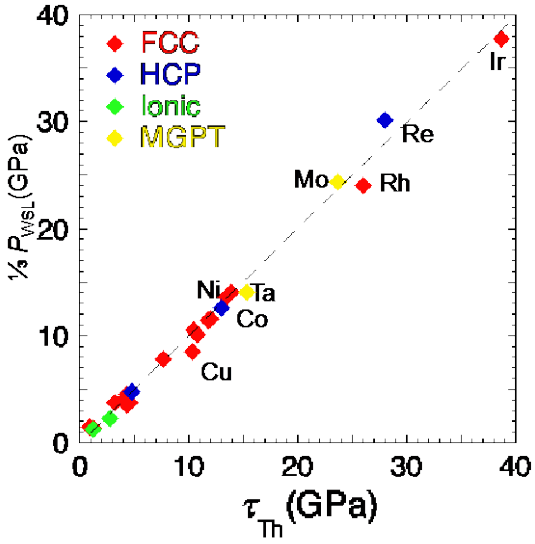

Figure 3. The variation of the weak shock limit threshold (⅓P_{WSL}) with theoretical strength for a range of close-packed metals and ionic salts. Strengths calculated using Frenkel formulation and for Ta and Mo using MGPT [11, 12]. Error bar on each point of order it's size so not reproduced here.

4. Discussion

The observations outlined above have wide-ranging implications for the use of computational and experimental tools. In particular the *finis extremis* and the mesoscale-microscale boundary define limits on an area of space in which a particular set of developed analytical tools may be applied. The code platforms have developed in different manners across the micro-/meso- boundary with particle interaction codes found at the microscale and continuum wave codes operating at the mesoscale and above. Molecular dynamics methods use an approximation to the wave-function (derived using density functional theory, DFT, to simplify description of wave-function) and neglecting electronic contributions to the energy [15]. On the other hand the continuum codes fit data at yield at the structural scale that is used to populate models for strength and equation of state behaviour at the mesoscale and above for simulations that may run to megabars. These codes can only qualitatively represent response in their present state unless fitted to results close to the application simulated, and thus advance in this arena calls for better consideration of the defect populations at different scales within the component materials. Further one must reformulate code platforms with consideration of the mechanisms that become necessary as one crosses scale boundaries in order that predictive power can be better ensured with these codes in the future. The problems come in definitions of quantities across the mesoscale boundary and in the formulation of particle and continuum systems within each scale.

5. Conclusions

This paper has considered nine orders of magnitude of length- and timescales and the same in pressure. It has concentrated on the space in which strength is defined and deformation may be described by analogy with the ambient state. This regime is the realm of *akrology*; that over which solid mechanics describes material response [6, 15]. For states in which loading has made flow steady,

local thermal equilibrium (LTE) has been achieved and propagating waves are steady within the regions that they sweep. Further the thresholds of static and dynamic behaviour converge with one another within materials as they deform. It is amazing that such a miscellany of accessible states with such a few simplifying thresholds can define the structures of planetary form that surround us. Further, the rich and varied behaviour observed in the weak shock regime homogenises with pressure as compression mounts dynamically or statically [16].

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