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Thresholds in Shock Response Across the Elements

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Abstract. Compendia of shock data have been assembled across national laboratories across the world. Previous work has shown a threshold in behaviour for materials; the weak shock limit. This corresponds to the stress state at which the shock is overdriven in a single front. Here the shock velocity-particle velocity data for elements and compounds has been systematically analysed to note discontinuities in the data. A range of materials show such features and the form of the discontinuity in each case is analysed. Some of these are found to correspond to martensitic phase transformations as expected whilst others are more difficult to classify. Particular groups within the elements show characteristic forms according to their groupings within the periodic table. Typical datasets are presented and trends in behaviour are noted for a range of elements.

1. INTRODUCTION

Fig. 1 a). shows a schematic of the levels at which transitions occur in a material under compression. In previous papers the existence of a boundary in behaviour has been described in which a threshold was overcome in the compression of condensed matter that related to bond strength within condensed elements [1]. This threshold, the weak shock limit (WSL), represents the transit in wave structure from an elastic wave followed by a front behind which inelastic deformation occurs, to a single shock rise to a Hugoniot stress within the material; the stress at the transition from the weak to strong shock regimes. This may be simply stated as a relation between wave speeds in the material; that the longitudinal elastic wave speed, c_L, becomes equal to the shock velocity, U_s, in the material. This threshold corresponds to the point at which the stress behind the front becomes equal to the theoretical strength of the element. A further physical interpretation regards the limit as the end of the region of inhomogeneous deformation that results from slip of elastic blocks. Material behaviour is dominated by the inelastic flow that accommodates the strain in a pulse. Operation mechanisms include slip and fracture to close defects present but also martensitic phase transformation and twinning which operate within this regime. All of these processes expend plastic work in the flow and increase the temperature behind the front, but it is only at the WSL (and above) that all processes are complete within it. Above the WSL flow is uniform with homogeneous nucleation of dislocations. In the strong shock regime the strength is maximized when matter is probed with some reload, strength is found to decrease with pressure only due to the thermal heating that occurs [2]. In this region jump conditions apply across the step front with homogeneous material behaviour. The shock front contains all operating processes with the flow behind it steady and the state in quasi-equilibrium since all compression processes are complete. The front itself obeys the Swegle–Grady laws with decreasing shock width with rising shock pressure and with the energy and kinetics of operating processes thus determining this length. Since times are short there is no mixing, so that whilst phases behave homogeneously, diffusion does not occur and release from the strong shock regime results in a microstructure where boundaries still exist and stacking difference across grains are preserved from the initial as-received state.

When compression increases in the strong shock state a threshold is eventually reached at which inner electron shells overlap and the electronic structure of the bonded element changes. This state is called warm dense matter in which whilst uncharged, electrons are localized away from nuclei [3]. Clearly valence electron bonding is not an appropriate description in such a state and much greater strengths are displayed since the potential rises rapidly with compression. This threshold has been dubbed the *finis extremis* in other work and lies between *ca*. 100 and 300 GPa according to the electronic density of states in each element or compound considered [4].

Discussion of theoretical strength began with the work of Frenkel and Orowan-Polanyi, and has been more recently extended [see 1]. The theoretical shear strength for the material (τ_{Th}) may be computed using a range of methods but one simple but powerful determination after Frenkel is given by the shear modulus $\mu/2\pi$.

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The correlation between ⅓σ_{WSL} and τ_{Th} is shown for *ca*. 40 elements and compounds for which shock and longitudinal wave speeds are available (Fig. 1 b). Each point represents a different element or compound and two (tantalum and molybdenum) have been shown with shaded regions spanning the simplest (Frenkel) estimates at one extreme to, at the other, the most modern and sophisticated quantum mechanics calculations. There are two groupings identified by the solid and dotted lines in the figure. The first fits the close packed FCC and HCP metals, the ionic solids and some alloys that are FCC or close to that structure such as Ni_3Al and stainless steel. A second fit (dotted line) may be found through a group of materials which are more open structured than those discussed above including BCC metals and amorphous non-metals. The fit-line through the open-structured materials has a gradient of 1.25±0.05 and lies above that for the close packed solids that have a fit gradient of 1.00±0.05. A more complete discussion may be found in [1].

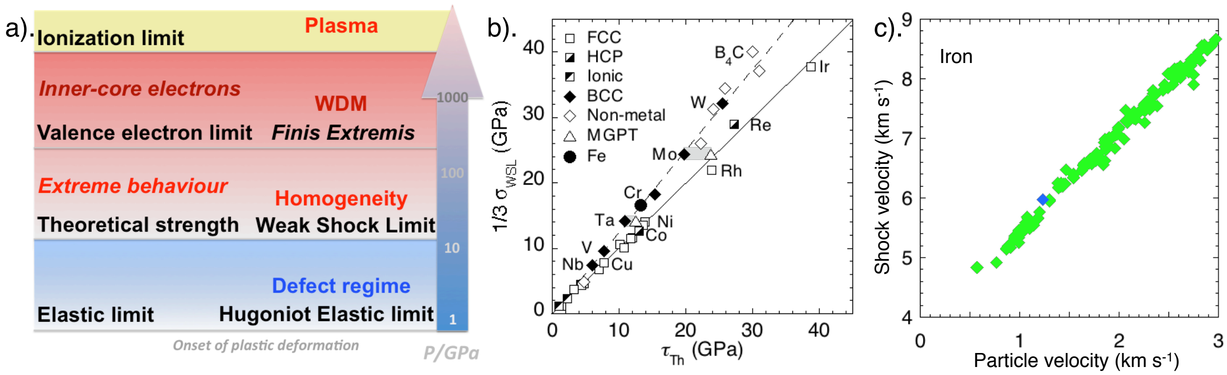

FIGURE 1. a). Regimes of behaviour for condensed phase materials; b). variation of the experimentally measured weak shock limit threshold with estimated theoretical strength; c). U_s-u_p for iron. Blue point at WSL [1].

Finally Fig. 1 c). shows U_s-u_p data for iron. A kink is seen which correlates with the WSL where U_s=c_L and occurs at *ca*. 60 GPa (blue diamond). Iron is the most studied of elements undergoing martensitic transformations both statically and under shock ($\alpha-\varepsilon$ transition at 13 GPa for instance) and thermodynamic transitions have also been extensively mapped because of its importance in planetary science for instance shock measurements of the melting temperature have shown it to start at 225±3 GPa [5]. One of interest concerns a change in magnetization to the non-ferromagnetic phase that occurs at 22.3 GPa (around one third of the WSL). This is a further indication of important electronic processes that occur at the WSL during loading as well as progression from hetero- to homogeneous behaviour at this level. This will be seen to occur for many elements across the periodic table.

2. MATERIAL RESPONSE IN DIFFERENT REGIMES OF BEHAVIOUR

2.1 Behaviour in compression across the WSL

It has been noted that actually few elements possess linear U_s-u_p relations; often overlooked when using the well-known approximation $U_s = c_0 + Su_p$ to simply describe shock behaviour. In this work we have systematically digitised the available shock data for the elements available in open databases and here review the shock velocity-particle velocity behaviour to identify trends. As with iron above it will be seen that many materials show a change in the shock parameter *S* at the WSL. Others show a change in *S* from a higher to a lower value (like iron) but equally change from lower to higher value in other cases. When this transit occurs at the WSL the cause is often difficult to ascribe.

Fig. 2. shows examples of elements that illustrate these behaviours. A principal feature of rare earths elements is those properties that depend on the occupancy of the 4*f* electron shell, from 0 (La) to 14 (Lu). Fig. 2 a). shows U_s-u_p behaviour in three metals; Praseodymium, Neodymium and Ytterbium. Each shows a concave form with an inflexion *ca*. U_s = 3 mm μs^{-1}. Many of the lanthanides show phase transformations; pressure, temperature and magnetic. However it should be noted that for both Pr and Nd the WSL of the materials lies almost precisely at these inflexions. Further, Ytterbium, at the other end of the period, has a lower transition stress again close to 2 GPa as seen. Cerium interestingly shows a different form to its shock behaviour locus with a convex form and point of inflexion at *ca*. U_s = 2.5 mm μs^{-1} (Fig. 2 b). This corresponds to a stress near 16 GPa in the element. There have

been some observations of a possible change in residual resistivity and superconducting transition temperature at *ca.* 16 GPa in cerium but there is no structural transitions found under shock that the authors have found at this pressure [6]. The data allow no definite conclusions at present but there may be evidence of phase transformations occurring related to stresses exceeding bond strengths in the materials and this may suggest the possible existence of a law-of-corresponding states for these elements at these thresholds at high pressure [6].

Finally Fig. 2 c) gives a schematic overview of the observed form of the U_s-u_p behaviour for elements across the periodic table. A red line on the table shows either a proportional behaviour (diagonal line), a lower followed by a higher *S* (double slope as in Pr, Nd, Yb above) or the converse (as in Cerium) where the slope goes from a higher to a lower value. Elements can thus be grouped into those with linear U_s-u_p, those where *S* increases and those where *S* decreases. It will be seen that the alkali metals and earths show linear behaviour whilst elements to left of Fe show generally *S* increasing with pressure after the WSL, whilst those to right show *S* decreasing. After Cerium following members of the Lanthanide series all show *S* increasing as one crosses the period. In summary the value of *S* (if it alters in higher pressure phase) generally increases as one crosses the table from Group 1 to Group 8. These trends follow the bonding and thus the coordination of the outer electron shell *s, p, d, f.*

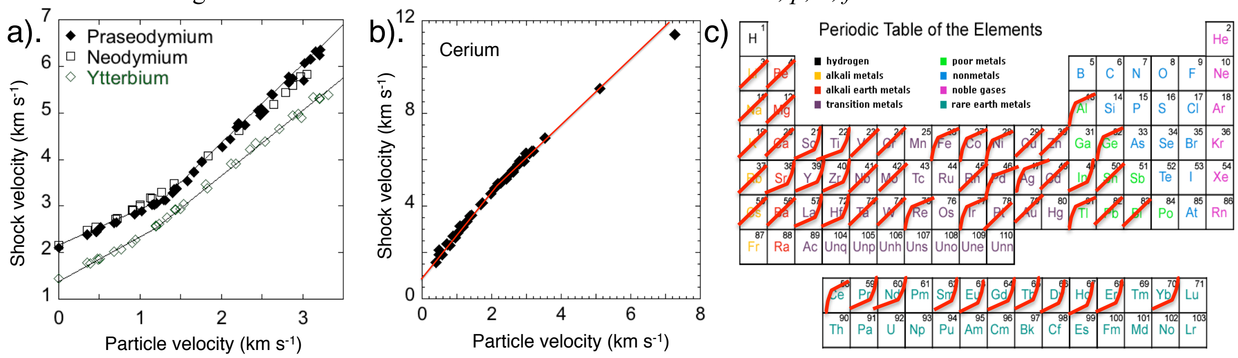

FIGURE 2. U_s-u_p data for rare earths; a). behaviour across the series; b). cerium; c). trends across periodic table.

2.2 The *finis extremis*; the transit to warm dense matter (WDM)

There is a transition from inhomogeneous to hydrodynamic behaviour at the WSL. Compression to higher loads results in the reorganization of electronic states and bonding exceeding consideration of purely valence electrons (the *finis extremis* FE). Here 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 undefined [1]. The regime between the yield surface and the FE defines *extreme* loading in what follows.

One indication of where the FE threshold lies comes from calculation according to electronic density of states calculations lies between *ca*. 100 and 300 GPa according to the element or compound considered. Here high compressions lead to new electronic correlations and closer atomic packing as compression proceeds [3]. These are *superextreme* states, of which the first dubbed Warm Dense Matter (WDM) ionizes at higher pressures to form a homogeneous plasma (Fig. 1 a). Thus the locus of compressed states (the Hugoniot) is expected to show different strength behaviour after this point. Strength may be simply related to the offset of the Hugoniot and the hydrostat (see [2]). Fig. 3 shows the response of three metals with calculated offset between Hugoniot and the hydrodynamic response (calculated from c_0 and *S* in the hydrodynamic region) for published data plotted as a function of pressure. This gives an indicator of the bound strength of the medium under shock. The red shaded areas bound the scatter and the points represent data collected using a range of experimental techniques and diagnostic developments over the past 50 years [7, 8, 9]. There is a rise in the deviation up to the WSL and then in each case a flat response up to a value at which deviations from hydrodynamic behaviour then become large.

This maybe due to an electronic transition in states as described earlier. However there are other possible explanations although these materials do not undergo martensitic or thermodynamic transitions at these pressures for instance Copper shock melts at 250 GPa, Tantalum at 300 GPa and Tungsten at 400 GPa [10, 11, 12]. Of course the accuracy of the measurements and deduction of the pressures obtained by various means becomes more uncertain as pressure increases but this effect would be expected to give a monotonic increase in Δ not a step change. Interestingly deviation occurs at around a pressure of three times the bulk modulus, $K/2\pi$, just as the transit to weak shock behaviour occurred at three times $\mu/2\pi$.

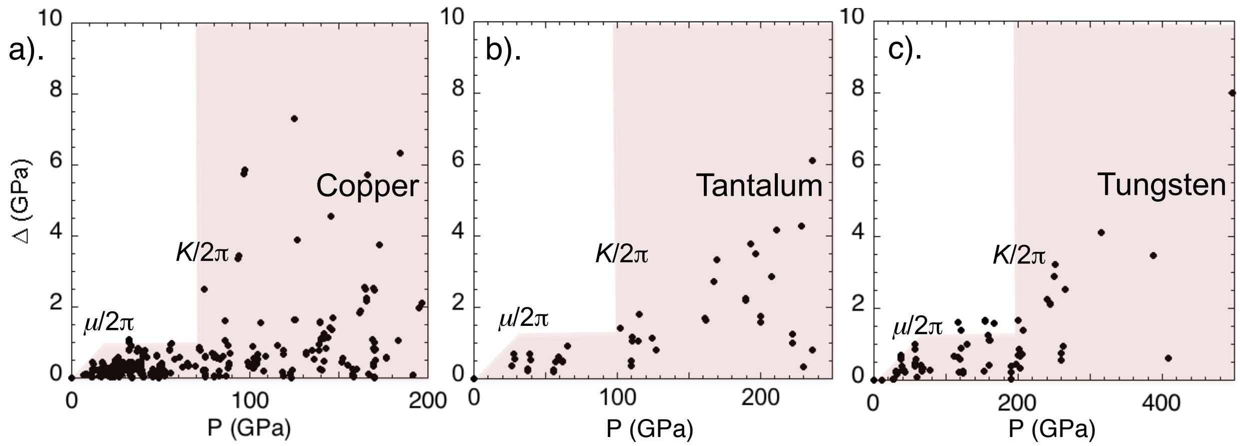

FIGURE 3. Deviation (Δ) of Hugoniot from hydrostat for Hugoniot data for a). Cu; b). Ta; and c). W [7, 8, 9].

5. DISCUSSION AND CONCLUSIONS

This work has presented some observations of the response of elements deduced from analysis of agglomerated shock data [7, 8, 9]. Analysis of the U_s-u_p behaviour for elements across the periodic table shows thresholds in behaviour. One of these occurs in many materials at the weak shock limit; the threshold above which there is a transit to a hydrodynamic, homogeneous state behind the front. This corresponds in many cases to a change in S for the material. Ruoff showed that $\partial K/\partial P = 4S$-1 (at zero p) and thus S follows the compressibility of a phase as pressure increases and in many cases there is change in S at the WSL [see 4]. This pattern across the periodic table shows that the electronic structure is key in determining the increase or decrease in compressibility. Further these transitions are reflected in elements' moduli and limits in compression are found that reflect macroscopic moduli μ and K.

Of course in a study of this sort it is not possible to access, assess and reanalyse every static and dynamic study in the literature for all of the elements in the condensed phase and the authors are sure that we have missed papers that explain our observations in some cases. However the data presented show that there is sufficient question over traditional interpretations of behaviour to justify further work to explain these trends.

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