Implementation of Hydrodynamic Simulation Code in Shock Experiment Design for Alkali Metals

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Abstract. Shock compression techniques enable the investigation of extreme P-T states. In order to probe off-Hugoniot regions of P-T space, target makeup and laser pulse parameters must be carefully designed. HYADES is a hydrodynamic simulation code which has been successfully utilised to simulate shock compression events and refine the experimental parameters required in order to explore new P-T states in alkali metals. Here we describe simulations and experiments on potassium, along with the techniques required to access off-Hugoniot states.

1. Introduction

The alkali metals are commonly considered to be “simple” at ambient conditions, and are well explained by the nearly-free electron model. At higher pressures these metals have been shown to depart from this simple behaviour and exhibit more complex, low-symmetry structures [1, 2, 3, 4]. Due to limitations in resistive and laser heating in DACs, the investigation of such exotic behaviour in alkali metals has been limited to moderate temperatures. There have, however, been several computational studies which predict transitions at higher temperatures than are inaccessible using static compression techniques [5, 6]. The use of dynamic compression techniques allows the study of these transitions in previously unexplored P-T regimes.

Shock compression generates states on a Hugoniot: the loci of P-T states that can be achieved with a single shock. Off-Hugoniot states can be accessed using ramp compression, were the ideal pathway is an isentrope [7], and the region between the Hugoniot and the isentrope can be explored with multiple shocks or ramps [8]. The Hugoniot and isentrope of potassium are shown in Figure 1, with the region accessible through multi-shock compression indicated by the shaded area. When combining multiple shocks in a multi-layered target, the complexity of the wave interactions is such that the final P-T states achieved must be determined with the aid of hydrodynamic simulations [9]. Such simulations are essential both in the choice of experimental parameters and also in aiding the interpretation of experimental data in real time.
The work presented here focuses on developing shock/multi-shock HYADES simulations in order to investigate unexplored regions of the P-T phase diagram of potassium. Potassium was chosen due to its structural similarities with Li and Na at high pressures, but with the phase transitions occurring at much lower pressures which are readily accessible at large-scale laser facilities. Preliminary laser compression data have been compared to the simulations presented here.

2. Methods

Simulations using the HYADES radiation hydrocode have been used to determine the laser compression parameters (pulse length, intensity, and double-shock pulse timing) and target parameters (ablator and sample thickness) required to compress potassium into previously unexplored P-T conditions. HYADES simulations utilise a Lagrangian mesh that moves with the target material [9]. Each zone in the mesh has a fixed mass and it is the movement of the mesh which determines the volume and the density of each zone through conservation of mass, energy, and momentum [14]. HYADES allows meaningful calculations to be executed rapidly with minimal computing expense which is advantageous in the planning of high shot-rate experimental campaigns and the interpretation of the results in situ.

The design of the target package is a crucial aspect of the experimental setup which must be optimised in order to access the required P-T conditions. Careful consideration of each target material’s shock impedance [13] must be taken into account. The impedance matching technique allows a low-impedance material of interest to be layered between two higher-impedance materials such that a series of reverberating compression waves ‘ring up’ between the two higher-impedance materials until pressure uniformity in the target is achieved. These interactions are illustrated in figure 2 [13]. The lower image shows the target design consisting of the high impedance ablator (I), the lower impedance material of interest (II) and the high-impedance window material (III), while the upper image illustrates the ringing up of a shock wave through a series of reflections in the material of interest. For the potassium targets we used Al as the ablator material, with windows of LiF, as these two materials are well impedance matched, thus ensuring that there are no significant pressure gradients within the sample at peak compression. The SESAME database was used for equation of state and opacity data for...
for Al, K and LiF [15].

The experimental work on potassium was conducted using the Janus laser at the Jupiter Laser Facility, LLNL, USA. This facility offers two Nd:glass (527 nm) laser beams which can provide flat-top pulses with energies up to 500 J and pulse lengths between 0.35 and 20 ns. A 1mm$^2$ phase plate was selected for use with pulses between 6 and 10 ns in length using varying energies.

3. Results and Discussion

Initially, single-shock simulations were used to understand the effects of a shock propagating through the multi-layer target package discussed above. This allowed the optimisation of the target parameters, laser pulse length and energy within the physical constraints of the Jupiter Laser Facility and the availability of materials. The effect of the ‘ringing up’ of the shock wave was determined, along with the length of pulse required in order to sustain compression through the ablator to the rear surface of the potassium. For a flat-top pulse length of 10 ns, a series of laser energies between 25 J and 175 J were simulated for a target consisting of 25 µm Al, 10 µm K and 500 µm LiF. These simulations showed initial pressures between 1 and 10 GPa in the K layer, with a subsequent jump to pressures between 2 and 17 GPa following the immediate re-shock from the K/LiF interface. After the ringing-up of the re-shocks between the high-impedance Al and LiF layers, the peak pressures in the K layer ranged from 4.5 to 32 GPa.

These simulations agreed well with the experimental data, as illustrated in Figure 3, which compares the experimentally-determined particle velocity in the K layer resulting from a 100 J, 10 ns flat-top pulse to the output from a HYADES simulation using the same parameters. The good agreement between the simulated and experimental velocity data means that the P and T obtained from the simulation (23 GPa and 2400 K) may be used to infer a location on a P-T diagram for the shock event (as shown on Figure 1).

![Figure 3](image)

**Figure 3.** The experimental VISAR trace from a single 100 J, 10 ns flat-top pulse shows good agreement with the particle velocity data produced by the corresponding HYADES simulation.

More complex, double-shock experiments were then designed to further extend the range of off-Hugoniot P-T conditions that could be explored. This was achieved by first varying the initial shock in the system to take the potassium to an on-Hugoniot P-T state, with subsequent secondary shocks and further ‘ring-ups’ taking the compression pathway away from the Hugoniot

![Figure 4](image)

**Figure 4.** The upper VISAR trace and pressure plot show the results of a simulated double-shock event (50 J, 10 ns pulse and 150 J 10 ns pulse) with a delay of 6 ns between pulses, while the lower plots show the results of the same setup but with a delay of 9 ns between pulses.
towards an isentrope. One important aspect of this design process is the relative timing of the two laser pulses, as illustrated in figure 4, which shows a double-shock simulation in which an initial 50 J, 10 ns flat-top pulse is followed by a 150 J, 10 ns flat-top pulse. Figure 4(a) shows a simulated VISAR trace and 4(b) shows the pressure distribution in the distance-time plane, for a 6 ns delay between the beginning of the first and second laser pulses. Figures 4(c) and 4(d) show the same information for a 9 ns delay between the laser pulses. In the case of the 6 ns delay, the first compression wave is overtaken by that produced by the second pulse before the former has fully propagated through the K layer and reached the K/LiF interface. As a result, the VISAR diagnostic used during the experiment to obtain the particle velocity at the K/LiF interface will be unable to identify the particle velocity resulting from just the first shock, and instead observes only the jump to the higher velocity resulting from the combination of the two compression waves. The loss of information about the on-Hugoniot state achieved by the initial shock means that the final P-T state is not obtainable from the VISAR data. However, for the 9 ns delay, the initial shock is able to propagate fully through the K layer before the second wave catches up, allowing the on-Hugoniot state achieved by the first pulse to be determined. The final P-T state produced by the second shock is then more easily determined.

4. Conclusions
HYADES has been used to plan a successful experimental campaign on shock-compressed potassium, by optimising target design and laser pulse parameters. It has proven to be an invaluable tool in the interpretation of the complex wave interactions, and the subsequent P-T states induced, in a laser-compressed multi-layer target. The results are directly applicable to our on-going campaigns on Li and Na.

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