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Numerical and experimental study of isentropic compression by laser irradiation

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The melting curves and Equation of State (EOS) of iron or iron alloys at the inner core boundary (330 GPa, about 5000 K) are still unknown and severally limits current earth modelling. In order to answer partly to these issues, we are investigating iron EOS using simple shock techniques and a double shock techniques to reach off-Hugoniot state and measurements. The French National Research Agency (ANR) is now supporting a research program grouping several laboratories including geophysicists called *SECHEL* (Simulating Earth Core Using High Energy Lasers).

Here we present the recent work done within this project that concerns numerical and experimental studies on the laser generated isentropic compression of iron. The experiments, performed in the past few years on the LULI2000 laser facility, used two different approaches: indirect reservoir technique (fig.1 top) and direct ramp-shaped laser pulse irradiation (fig.1 bottom).

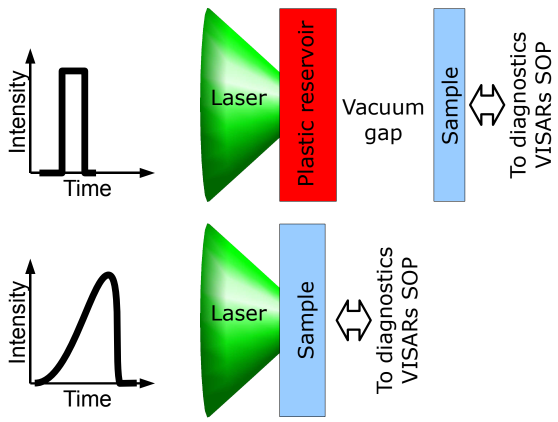

Figure 1: Laser shape and experimental setup for the reservoir technique (top) and the ramp compression (bottom).

These doesn't include plasticity or the kinetics of the phase transformation. To better understand the compression wave, a second step has been done by coupling this simulation with molecular dynamics simulation to reproduce and analyze microscopic effects in the studied material. This is a multi-scale approach to simulate matter in these conditions: the ramp of compression wave trajectory of the hydrodynamic simulation is used as a piston to push a molecular dynamics simulation (done using up to 10 million atoms with the STAMP code) on the same longitudinal and temporal scales of the experiment (some microns and ~ 1 ns). This

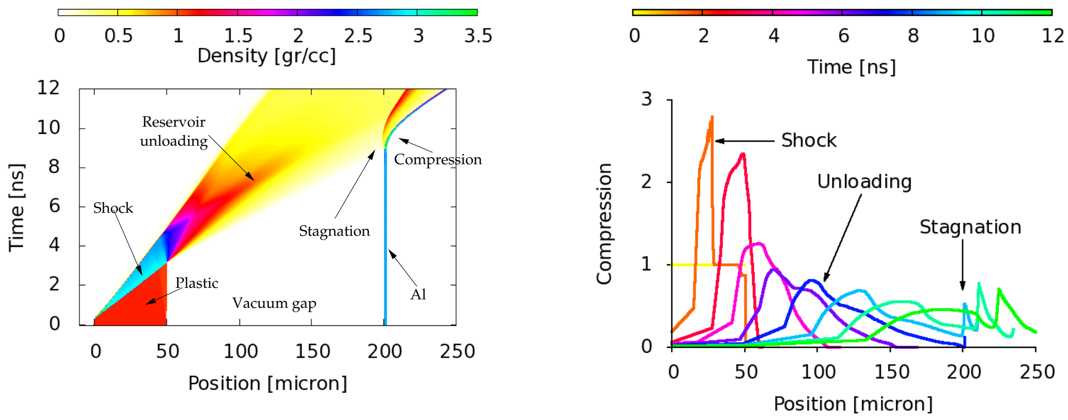

Figure 2: Reservoir technique: hydrodynamic simulation, on the left the density and on the right the compression (laser comes from the left).

a key point to have a complete picture of the experiment since the hydrodynamic approach doesn't include the underlying mechanism of the kinetics of the phase transition of the material.

The figure 2 shows a radiative-hydrodynamic simulation of the reservoir technique. Starting from the laser side (left on figure 2), the target is composed by a first layer of 50 μm of plastic (called *reservoir*) followed by a 150 μm vacuum gap and then we have the 2 μm foil we want to investigate. The laser interaction (intensity: 10^{13} W/cm^2, time:4 ns), generates a strong shock in the reservoir target that unloads in vacuum adiabatically and accumulates over the sample foil generating an isentropic compression. The simulation shows an acceleration of the foil corresponding to an almost constant value of $\sim 7\frac{\text{km}}{\text{s ns}}$. This parameter is important as it is used to simulate the evolution of the compression wave in the foil in the molecular dynamics simulation as a simple mechanical piston.

We present in figure 3 the experimental results of a sample shot. We show the evolution of the rear side velocity of a 10 μm iron foil accelerated by the reservoir technique. As most of the laser energy is lost during the laser interaction with the plastic reservoir, we cannot achieve a very high velocity. In fact, as the rarefaction wave come back into the sample, to the front surface, the foil reach a fairly constant low pressure and is no more compressed but just pushed and accelerated (with a good agreement with the simulation, fig. 3).

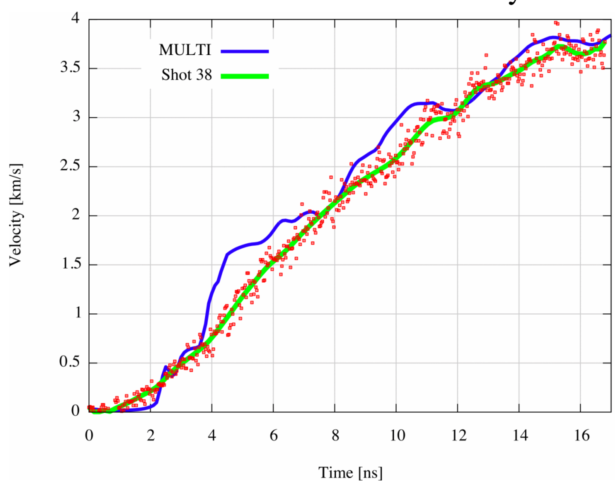

Figure 3: Rear side velocity of a 10 μm foil compressed with the reservoir technique compared to the hydrodynamic simulation.

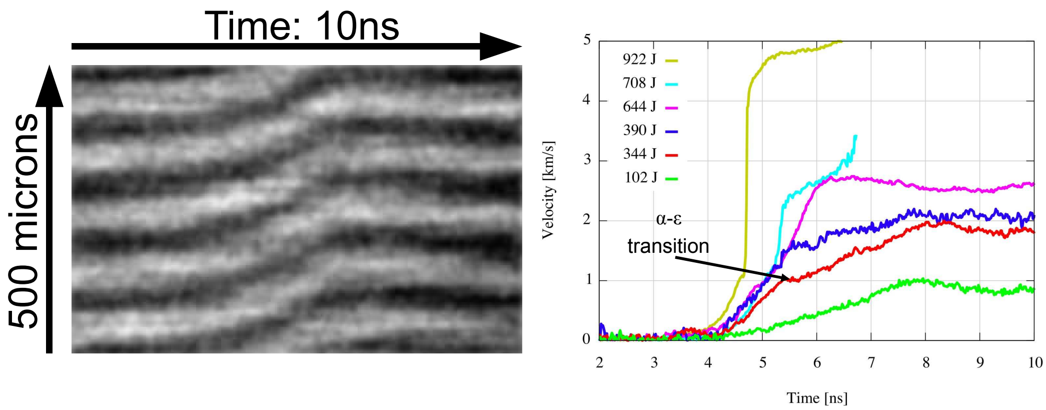

Figure 4: Pulse shape technique. Left: VISAR image. Right: Experimental result.

The simulation shows that the compression wave is not affected by the rarefaction wave just for the first 3-4 ns; after that time the foil reaches a constant low pressure even if the maximum velocity recorded is $\sim 3.5\mathrm{km/s}$.

For the ramp shaped technique the mechanism is simpler: we increase smoothly the laser intensity on target over 4 ns to reach a maximum and as result, we get a compression wave propagating inside the material without shock formation.

Since the laser attacks directly the target care must be taken in the choice of the target thickness to avoid any preheating of the material before the compression wave arrives. We choose to use 10μm iron foils since predictions from calculations shows no preheating effect due to the laser X-rays over 5μm of target.

The LULI2000 facility has a built-in pulse shape technique that can give an arbitrary pulse shape over 4 to 5 ns. In figure 4 we show the rear side velocity of the sample for different laser intensity (pulse shape: triangular profile in time). By increasing the energy of the laser on target, we see that we achieve a smooth compression with a maximum velocity that increases with the laser energy. We see that for high energy (yellow line), the compression is followed by a shock. As recently observed we have the alpha epsilon transition at a velocity higher than nominal (visible as a shoulder in the measured velocity $\sim 1\mathrm{km/s}$) due to the fact that we're doing a dynamic compression of the matter and the signature of the transition is blurred by the fact that we're registering the target rear side velocity rather than the in situ velocity.

This is just a preliminary experiment that shows the facility capabilities, the next step wil be to add a rear side transparent window (sapphire) to avoid the interaction between the compression wave and the relaxation wave that occurs at the rear side of the material and access with the VISAR the in situ particle velocity.

One of the key point to get an EOS from the VISAR measurement is the so called *Backward* *integration*. It is important to know the history of the rear-side velocity to integrate the equation of motion in order to obtain the stress-compression relation. This is done by assuming a perfect elastic response of the material. Experimentally however the presence of the elastic-plastic transition of the material and/or a phase transition, will lead to an entropy jump that needs to be controlled. We decided to couple the hydrodynamic results of the material compression to a molecular dynamic (MD) simulation. To evaluate the effect of the elastic-plastic transition on the BI we used a test-bed material (aluminium using an EAM potential) that doesn't have ant solid-solid phase transition but just the elasto-p

In figure 5 we show the differences between pure hydrodynamic model (red line) versus preliminary molecular dynamics simulation (blue line). We show the rear side velocity of a 1 μm aluminium foil compressed by a piston with a constant acceleration of 7 km/s/ns, the same for both simulations (black line). As we can see the small peak corresponding to the elastic-plastic transition that occurs at 2 km/s completely neglected in the hydrodynamic model. This means that the lagrangian sound speed that we can infer around and above that region, will be wrong and the BI scheme will be partially affected by this transition and wil lead to some uncertainities in the EOS obtained by the BI technique. For Al this elasto-plastic transition is quite small and can be neglected, but this phenomena will be much more important in case of a phase transition and the dynamics of the phase transition will have to be taken into account to apply the BI algorithm.

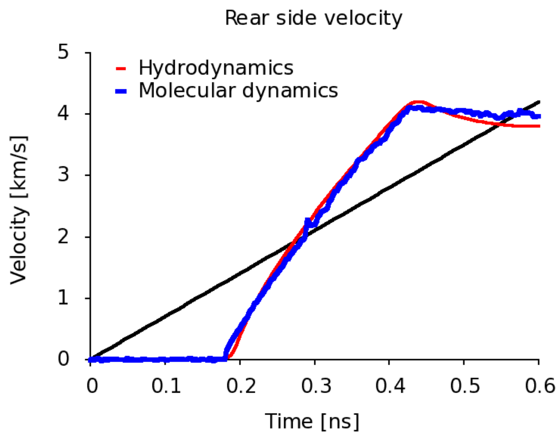

Figure 5: MD (blue) compared to Hydrodynamics (red): rear side velocity of an Al foil (1 μm) compressed by a piston (black line).

In conclusion, we have summarized in this paper the ongoing program supported by the ANR *SECHEL* to simulate and reproduce in the laboratory the isentropic compression of iron. We have reported the first experiments done at LULI on the iron compression by laser interaction with two different techniques (reservoir and pulse shaped) and we have shown a good agreement with hydrodynamic simulations using a known EOS (SESAME). For the reservoir technique, we have also shown the possibility of a multi-scale approach involving both hydrodynamic codes and molecular dynamics to uncouple the foil compression from the laser interaction. These simulations point out some major problems of the *backward integration* model to infer the EOS from the VISAR measure. T. Vinci and G. Morand would like to acknowledge the support of the french ANR programme ANR-07-BLAN-0239.