Shock-induced elastic, plastic and polymorphic transformations in iron films by picosecond laser pulse

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Introduction

An analysis of experimental and numerical studies of laser shock waves initiated by a picosecond pulse in iron is studied. A series of experiments were performed with different films width. A pump-probe technique provides free surface velocity histories. High deformation rate is a peculiarity of this research. The extremely short duration of the action of a mechanical load makes it possible to realize deeply metastable states of matter, far from equilibrium, and to study the behavior of various materials at extremely high deformation rates. The alpha-epsilon phase transition pressure value of 13 GPa very accurately determined by shock-wave experiments in iron with submicrosecond loading.

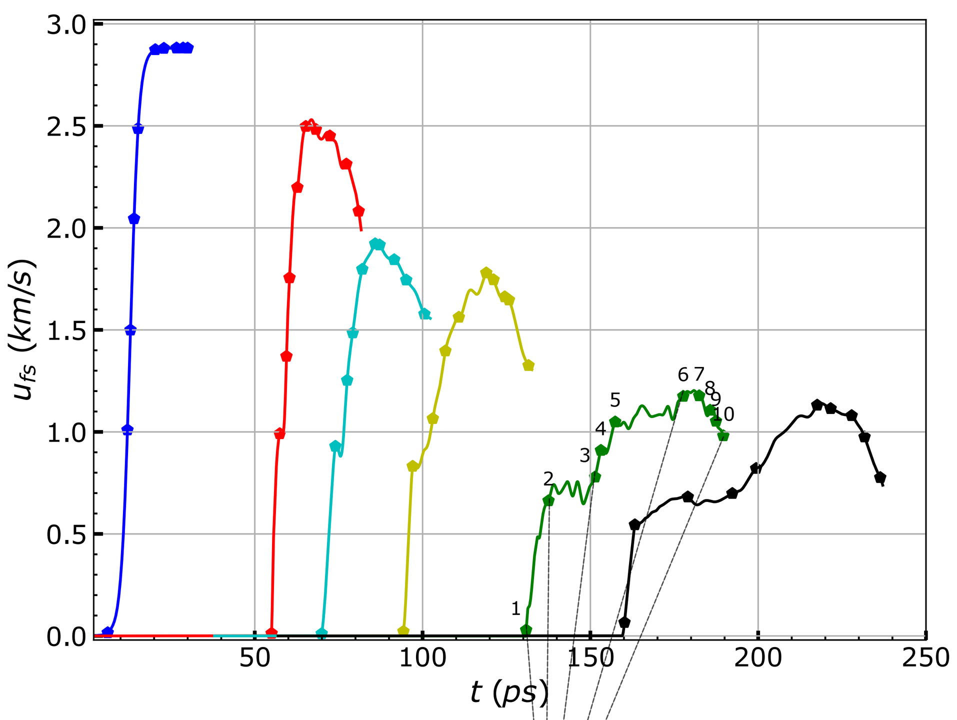
In this research, stress-strain diagrams are calculated with a lagrange inverse analysis technique [AidunGupta1991]. Inferred stress-strain diagrams are applied for understanding how the strain rate affects elastic-plastic and polymorphic transformations in iron. Molecular dynamics simulation assisted by 2T-hydrodynamic calculation validates theoretical approach for the inferred stresses-strain.

John B. Aidun and Y. M. Gupta Analysis of Lagrangian gauge measurements of simple and nonsimple plane waves. Journal of Applied Physics 69, 6998 (1991)

Inverse analysis technique

The main idea is in Lagrangian form of mass and momentum equations where right hand side depend on $u = u(t, h)$ and initial density $\rho_0 = 7.874\ \mathrm{g/cm^3}$

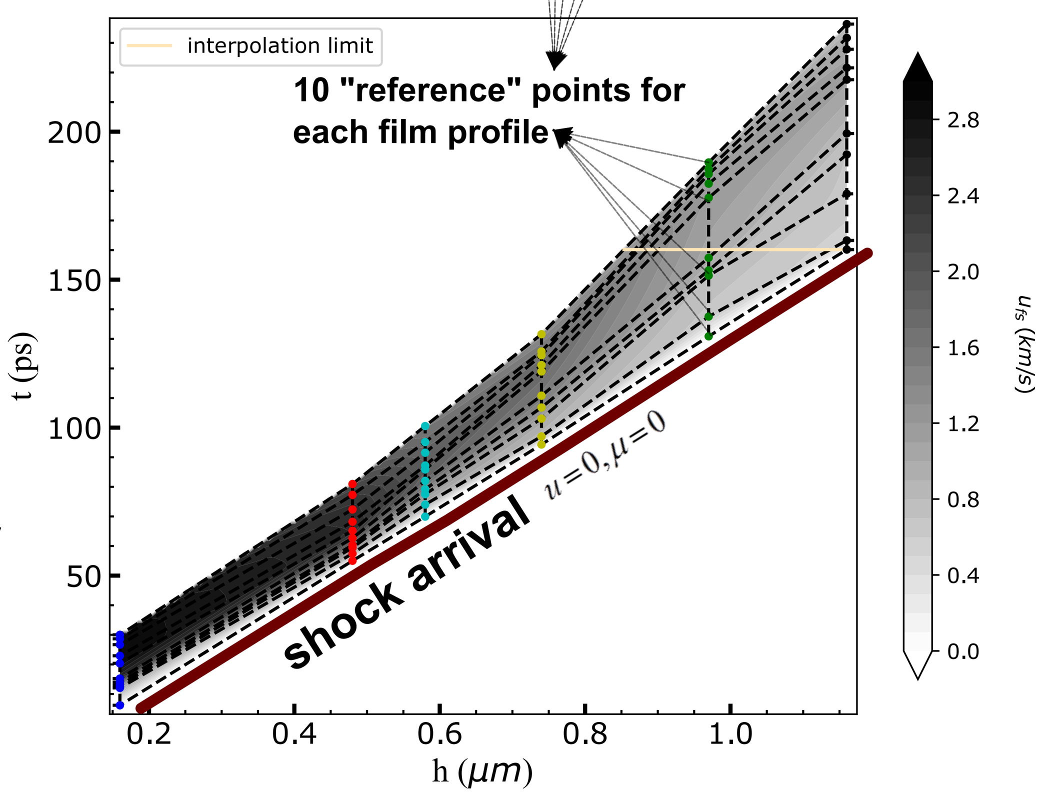
$$\frac{\partial \sigma}{\partial h} = -\rho_0 \frac{\partial u}{\partial t}$$
$$\frac{\partial \mu}{\partial t} = -\frac{\partial u}{\partial h}$$
$$\sigma = -p_{xx}$$
$$\mu = 1 - V/V_0$$



Set of film h: 160, 480, 580, 740, 970 and 1160 nm free surface velocity profiles are doubled mass velocity profiles

$u = u(t, h)$ defined with linear piecewise intepolation using 10 reference points at each profile

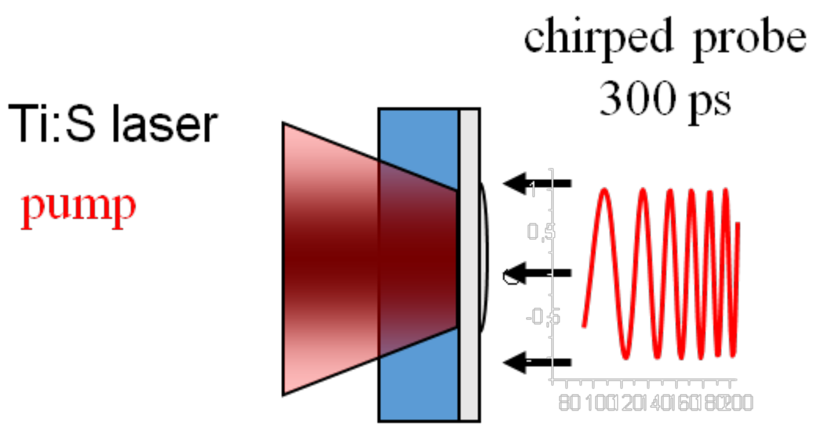
Numerical derivatives of defined function are integrated along horizontal (for stress) and vertical (for strain) are integrated for chosen set of "reference points"**



$$\sigma(t,h) = -\rho_0 \int_{h_b}^{h} \frac{\partial u}{\partial t}(t, h_1)\, dh_1$$ Finite difference derivatives approximation

$$V(t,h)/V_0 = 1 - \int_{t_b}^{t} \frac{\partial u}{\partial h}(t_1, h)\, dt_1.$$ Numerical integration with Quadpack library***

Experiment description



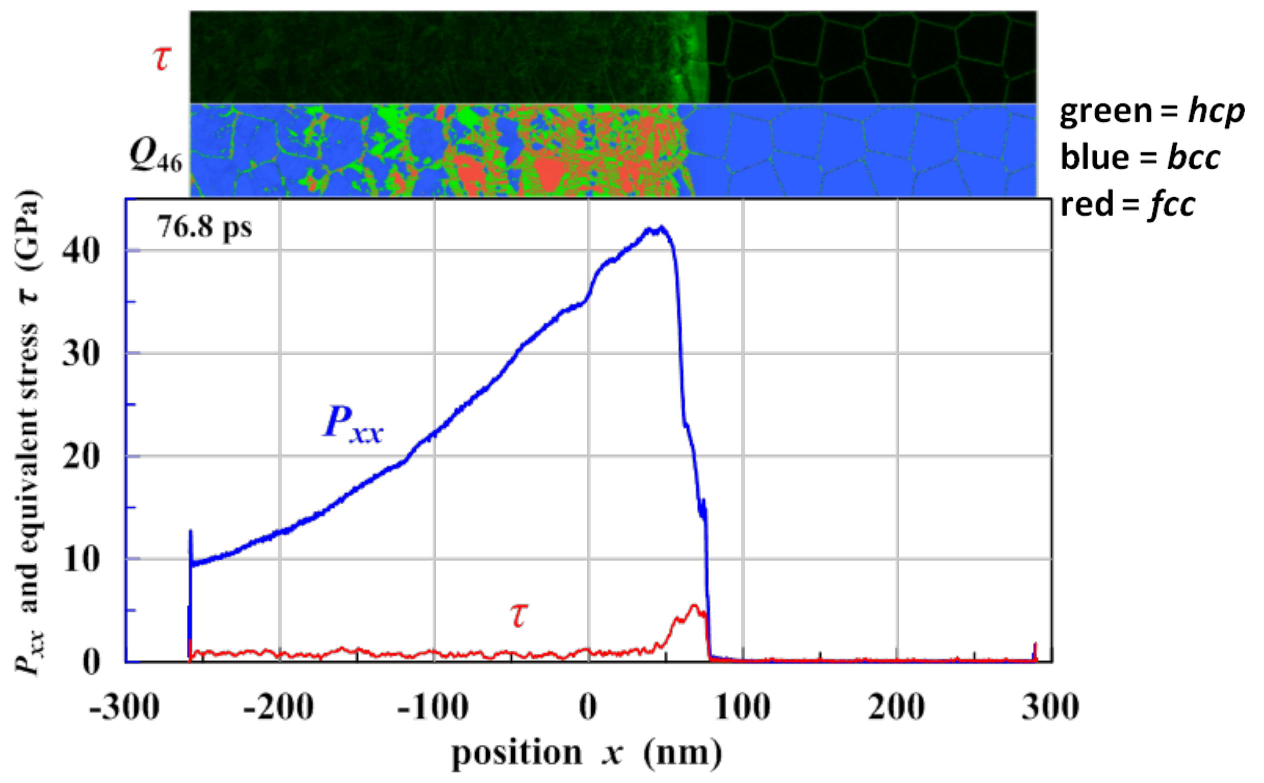
Iron films deposited by the magnetron method on glass substrates 150 μm thick. The source of heating and diagnostic pulses was a titanium—sapphire laser system. The duration of the heating pulse was 1.2 ps, wavelength 795 nm. An incident energy density at the center of focal spot is about 3.4 J/cm^2.

Chirped 300 ps probe pulse with linear frequency modulation and spectral width 40 nm provides
- Detected range 0-240 ps
- Temporal resolution 1ps
- Lateral spatial resolution 2 μm
- Displacement accuracy 1-2 nm
- Whole free surface displacements profile measurment with a single laser shot!

S. I. Ashitkov, V. V. Zhakhovsky, N. A. Inogamov, P. S. Komarov, M. B. Agranat, G. I. Kanel. AIP Conference Proceedings 1793, 100035 (2017)

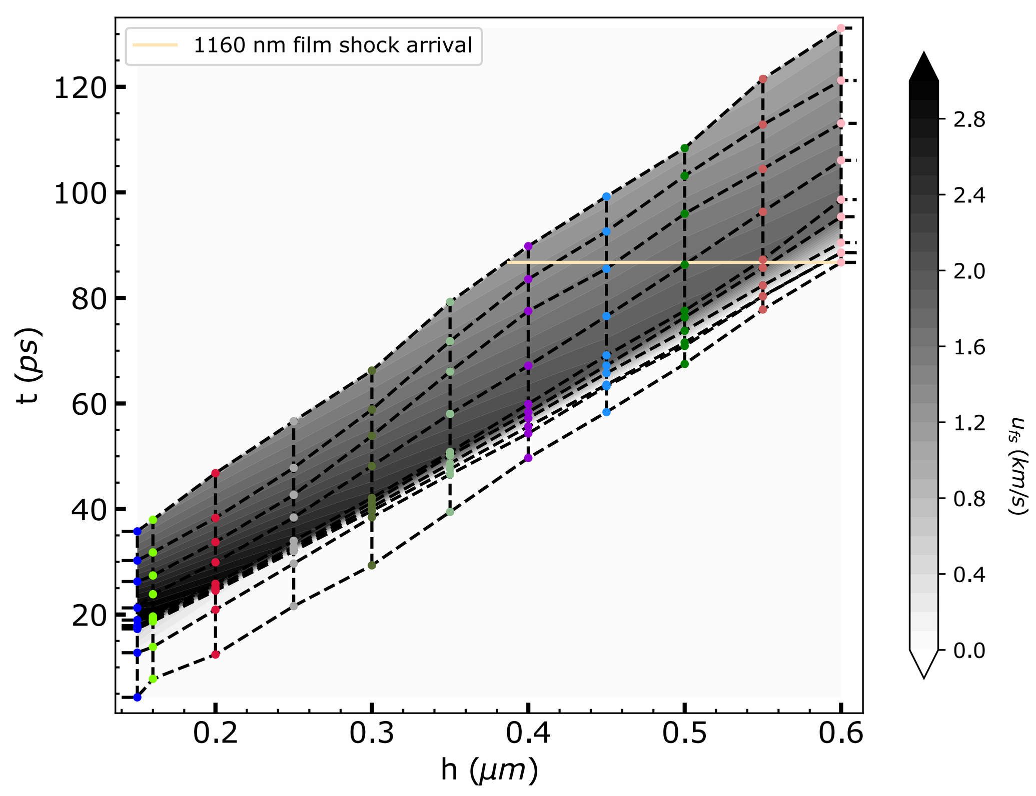
MD simulation and validation of inverse analysis technique

MD simulation provides full information about selected Lagrange particles h=150,200,...600, 160 nm
Sample dimensions 590x60x10 nm

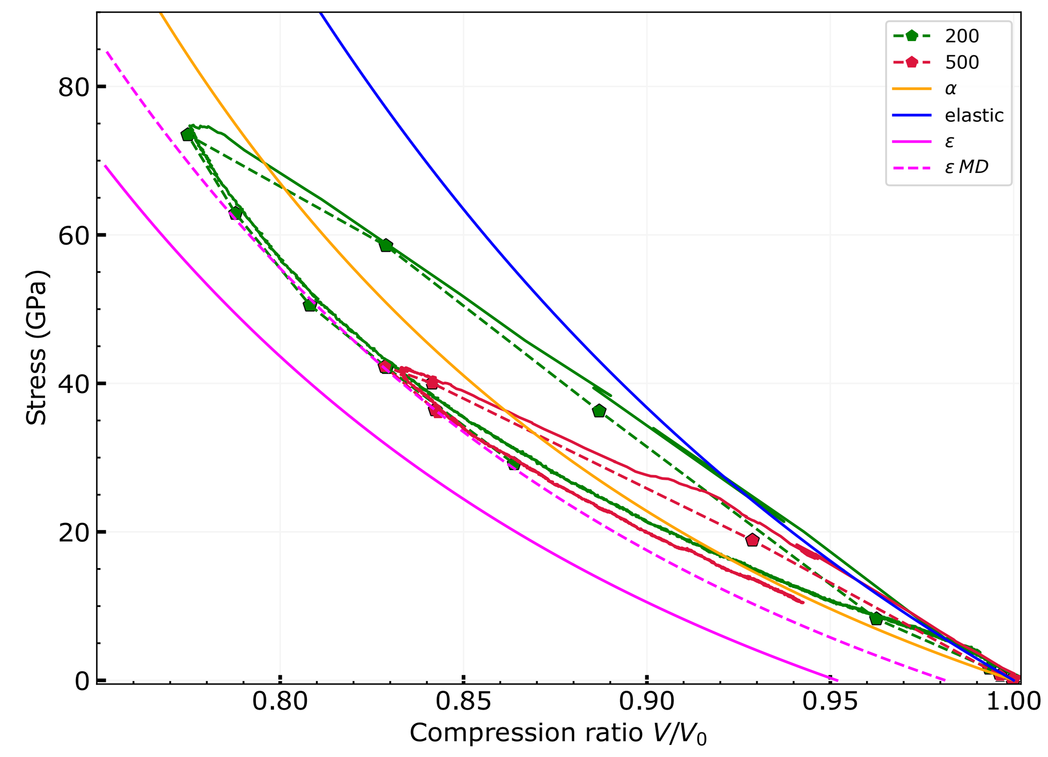


30 million atoms 590x60x10 nm polycrystal iron sample under piston pulse inferred from two-temperature hydrodynamic modeling.
The polycrystal is randomly oriented set of single crystals generated with Voronoi tesselation.

Approximation of $u = u(t, h)$ by the series of $u_{fs}(t) = 2u(t)$



Recovered stress-strain diagram: solid pathes from MD simulation dashed pathes from inverse analysis

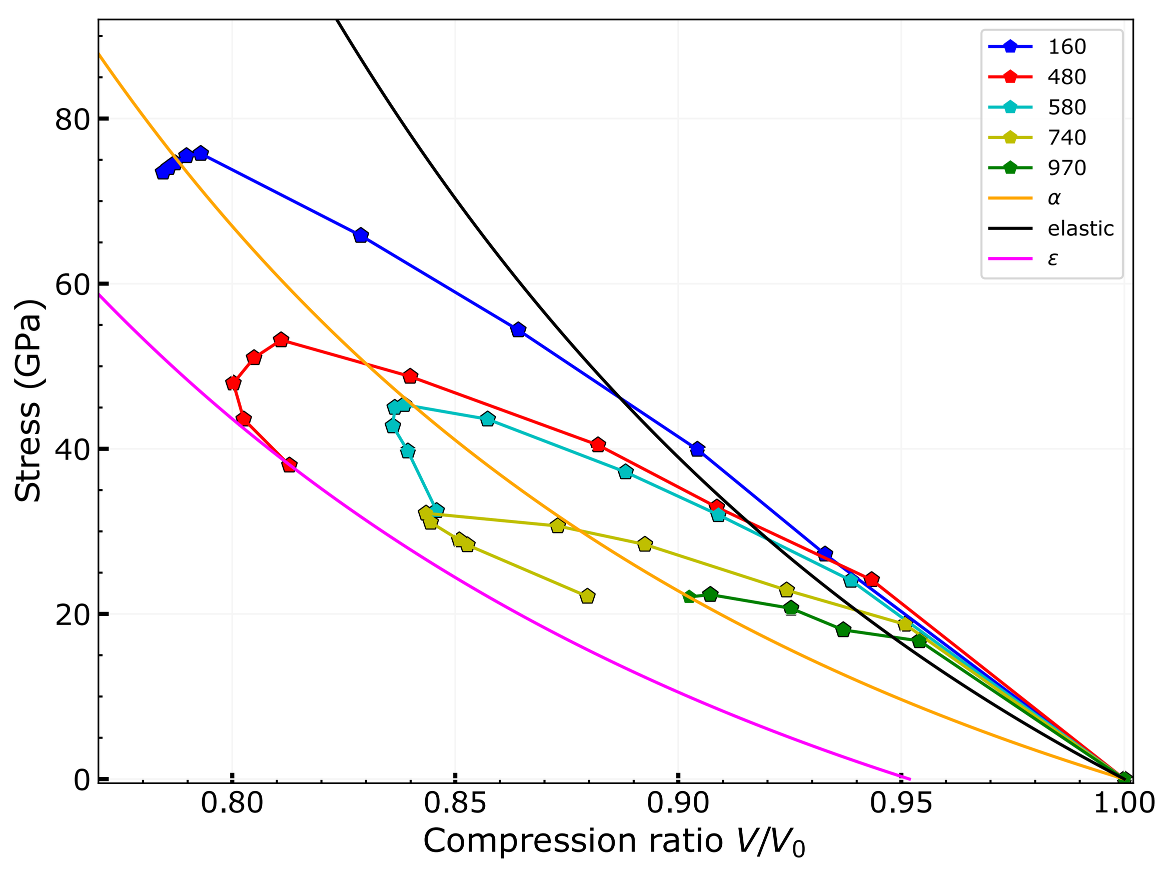


11 particles with h=150, 200, …600 and 160 nm are used
10 "reference"** points at each profile
On the right, shock Hugoniots of iron in elastic, alpha and epsilon phases are shown. Dashed Hugoniot of epsilon phase from MD simulation differs with experimental, because it's initial density prediction discrepancy from interatomic potential.

Results

Stress and strain could be obtained for all except the largest width 1160 nm and only part of 970 nm film, because interpolation limit (see above u(t,h)).

It was observed that the alpha-epsilon phase transition is completed in the unloading wave.



Conclusions

The analysis of the experimental data (the dependences of free surface velocity on time) for the laser shock in iron film is presented.
A series of profiles approximation procedure is developed.
This analysis makes it possible to determine the profiles of density and longitudinal stress from the experimental data. Profiles are projected onto the stress-strain phase diagram to observe alpha-epsilon phase transition.

References

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Jonathan C. Boettger and Duane C. Wallace. Metastability and dynamics of the shock-induced phase transition in iron. Phys. Rev. B, 55:2840–2849, Feb 1997.

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