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Dynamic properties of nickel−titanium alloys

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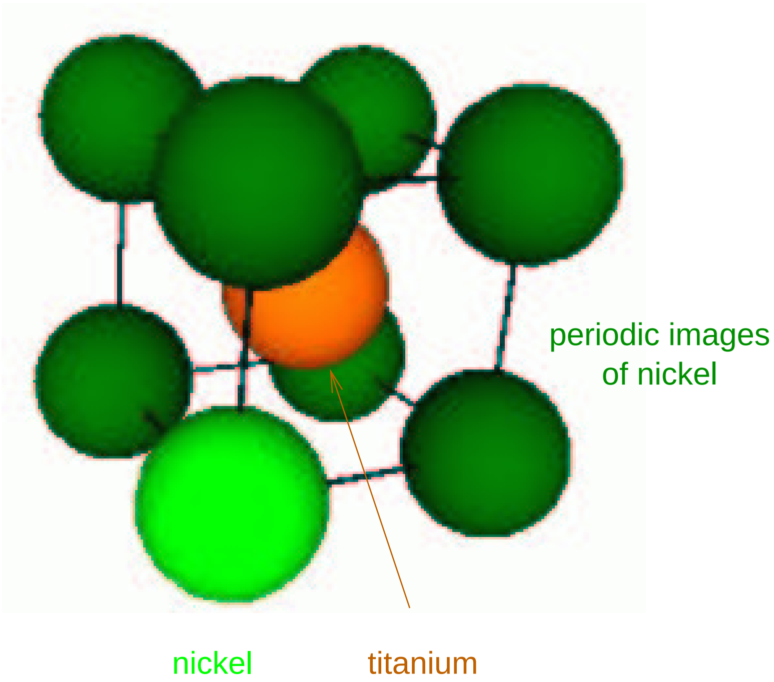
Abstract

The shock response of near-equiatomic NiTi alloys has been investigated to support studies of shock-induced martensitic transitions. The equation of state (EOS) and elasticity were predicted using ab initio quantum mechanics. Polycrystalline NiTi samples were prepared with a range of compositions, and thickesses between about 100 and 400 μm. Laser-driven flyer impact experiments were used to verify the EOS and to measure the flow stress from the amplitude of the elastic precursor; the spall strength was also obtained from these experiments. The laser flyer EOS data were consistent with Hugoniot points deduced from gas gun experiments. Decaying shocks were induced in samples, by direct laser irradiation with a variety of pressures and durations, to investigate the threshold for martensite formation.

Quantum mechanical calculations

Fairly simple predictions of thermodynamically complete equation of state and elasticity; method used before for other materials.



3D quantum mechanical calculations of electron ground states.

Nucleus + inner electrons represented by ab initio pseudopotentials.

Periodic boundary conditions: infinite crystal.

Schroedinger equation solved for outer electrons.

Exchange/correlation: local density approximation (LDA)
+ generalized gradient approximation.

Plane−wave basis set; 1000 k−points and 50 iterations to convergence.

Calculations repeated at different compression and strain,
predict frozen−ion cold curve and elastic constants vs compression.

NiTi: considered CsCl (B2) structure only, i.e. estimate of equation of state ignoring phase change energies etc.

Pseudopotentials for Ni and Ti were previously shown to give reasonable estimates of properties of elements.

Aside: mixture models for compounds

Common procedure for estimating unknown EOS: average EOS of constituents.

Mechanical equilibration of independent constituents: find $\rho_i(p)$:

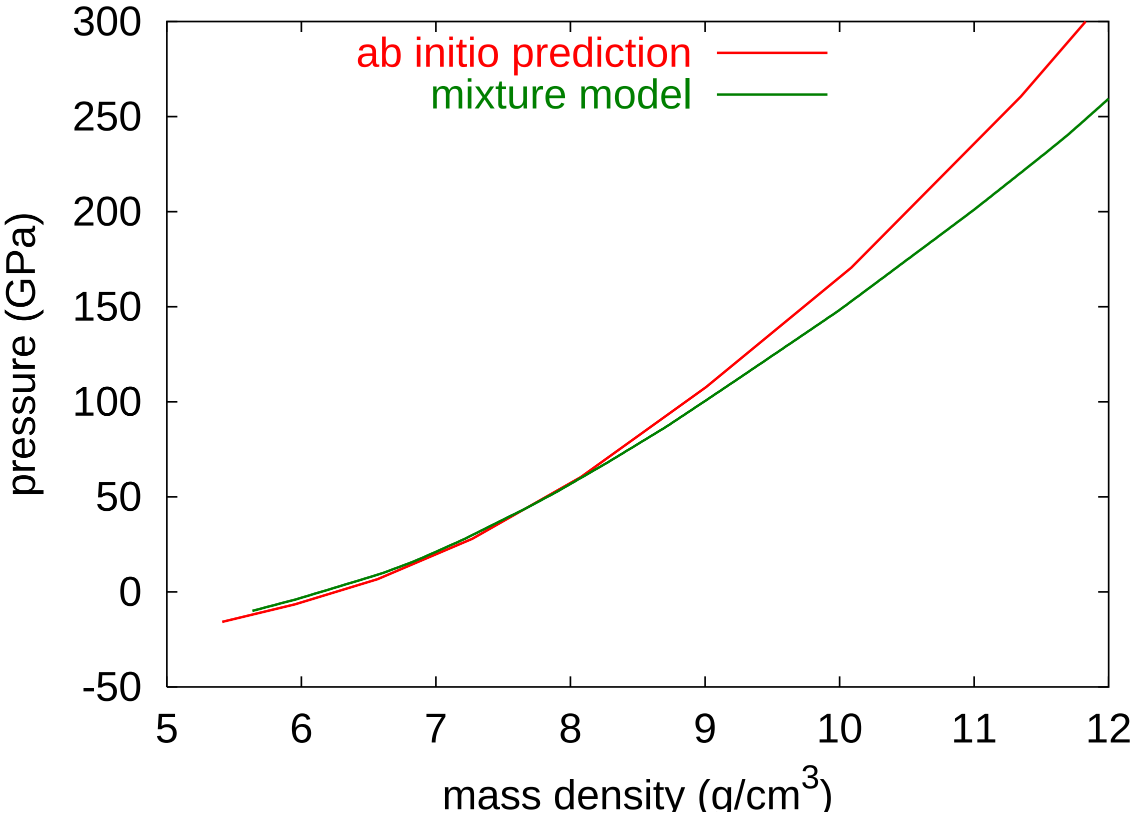
$$\bar{\rho} = \sum_i f_i \rho_i$$

f_i are volume fractions:

$$f_i = \frac{\mu_i}{\rho_i} \left[\sum_j \frac{\mu_j}{\rho_j} \right]^{-1},$$

μ_i are mass fractions from composition, number N_i and mass m_i:

$$\mu_i = \frac{N_i m_i}{\sum_j N_j m_j}.$$



In general, quantum mechanical predictions of actual composition are preferable to over−simplistic mixture models.

Theoretical Grueneisen EOS

Decomposition of EOS:

$$\begin{aligned} p(v,T) &= p_c(v) + p_e(v,T) + p_l(v,T) \\ e(v,T) &= e_c(v) + e_e(v,T) + e_l(v,T) \end{aligned}$$

Grüneisen approximation (cold curve as reference):

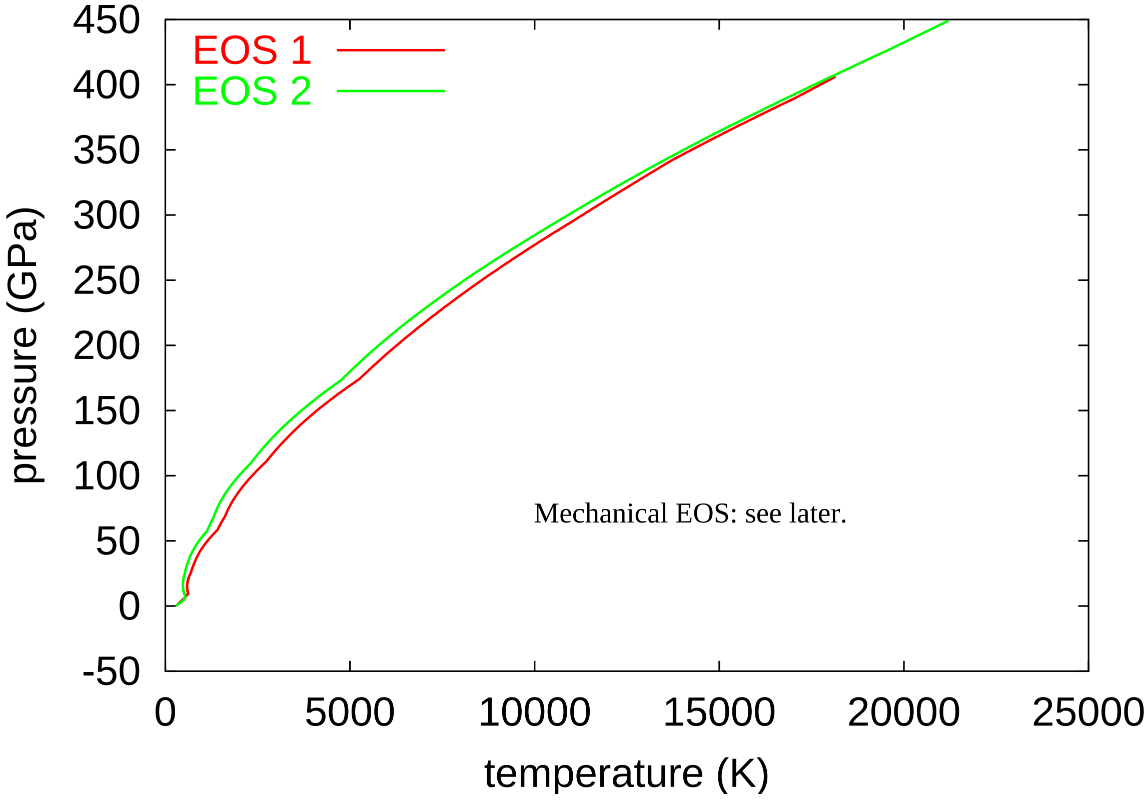
$$\begin{aligned} e(v,T) &= e_c(v) + \int_0^T c_v(v,T')\,dT' \\ p(v,T) &= p_c(v) + \int_0^T \frac{\partial}{\partial T'} \left\{ \frac{\Gamma(v,T')}{v} [e(v,T') - e_c(v)] \right\} \Bigg|_v dT' \end{aligned}$$

where c_v is total specific heat capacity $\partial e/\partial T)_v$; assumed $3k_B$/atom.

Dugdale-MacDonald relation used to estimate $\Gamma(v)$ on the cold curve:

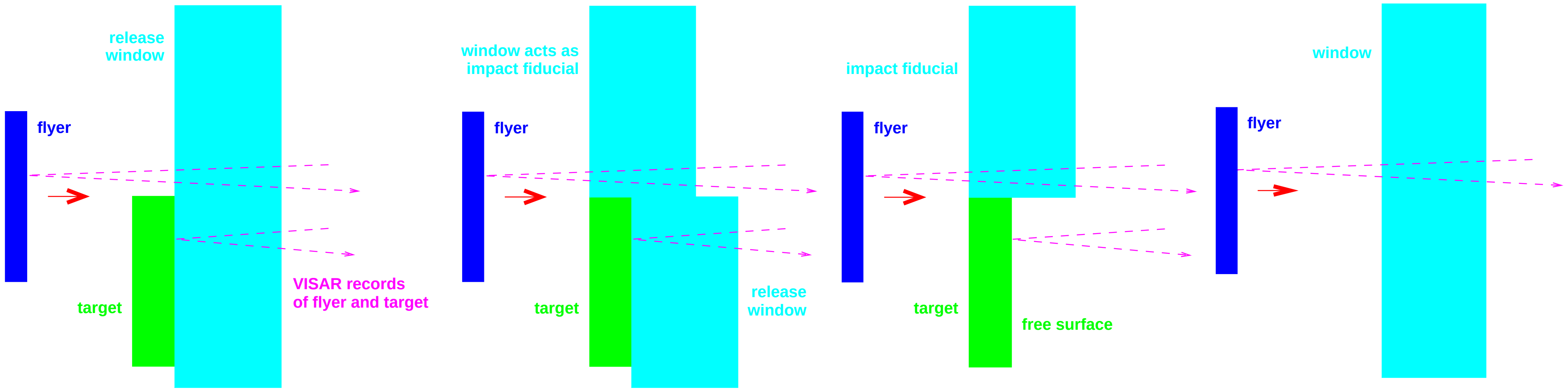
$$\Gamma(v) = -\frac{v^2 p_c''/2 + v p_c' + p_c/9}{v p_c' + 2p_c/3}$$

Thermodynamically complete EOS tabulated in SESAME format and fitted with cubic Grüneisen mechanical EOS for convenience. To investigate sensitivity to calculation of $\Gamma(v)$, generated EOS with different fits to cold curve: 2-point exponential fit (“EOS 1”) and four point quadratic fit (“EOS 2”).

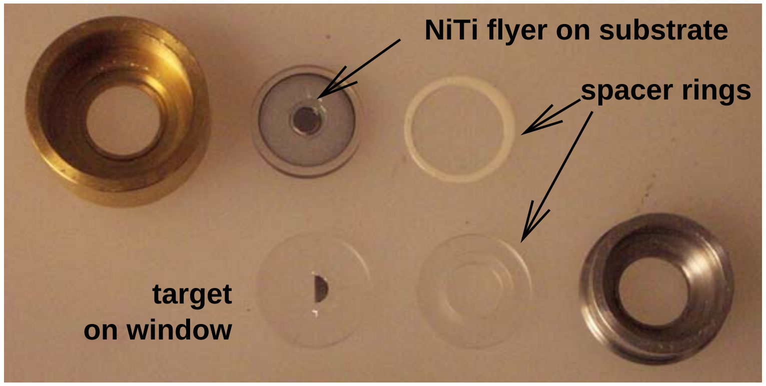


Laser−driven flyer experiments

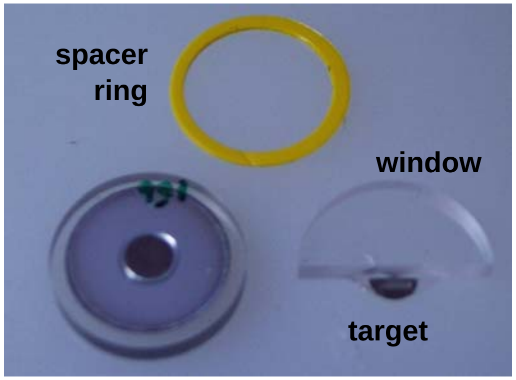
Used to verify/refine EOS, measure strength. Several designs used to optimize for NiTi:



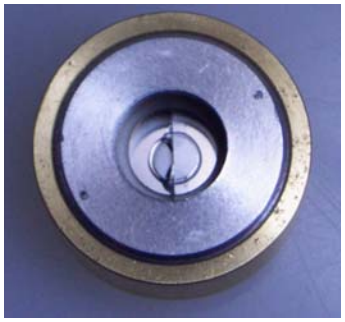
Horizontal scale exaggerated



Samples: 100 to 400 microns
by 5 mm diameter.

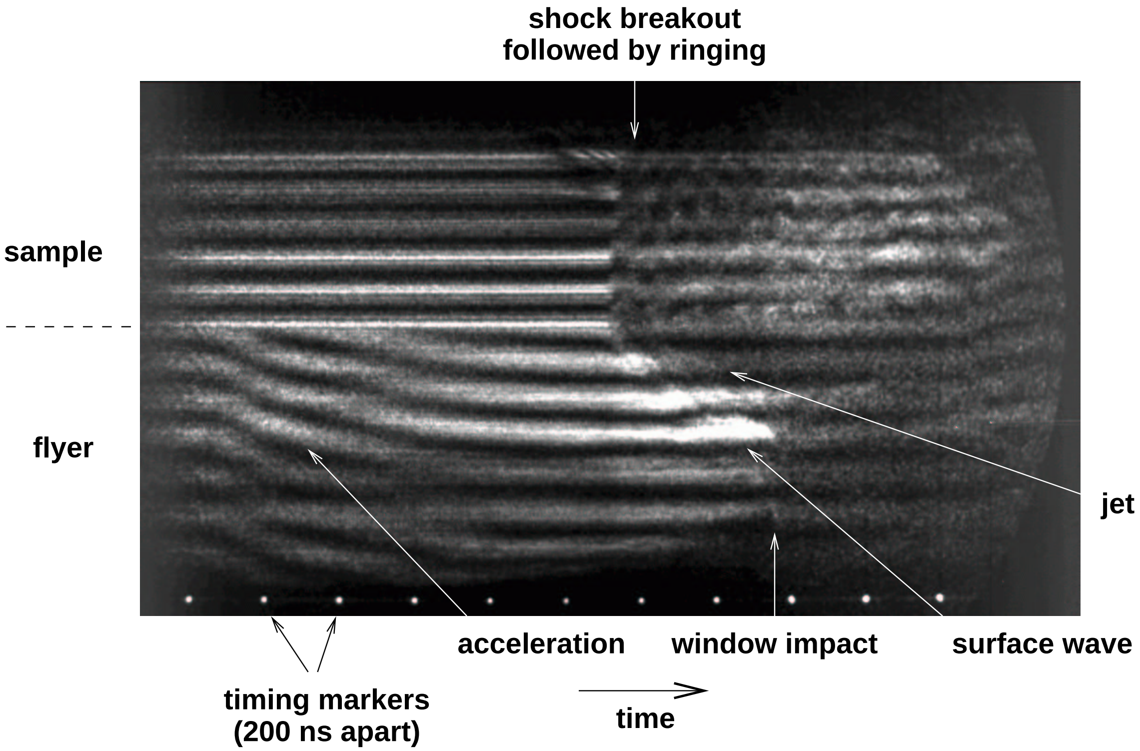


Launch system: TRIDENT laser
at 1054 nm wavelength, 600 ns pulse.
Energy delivered through substrate
to accelerate flyer.

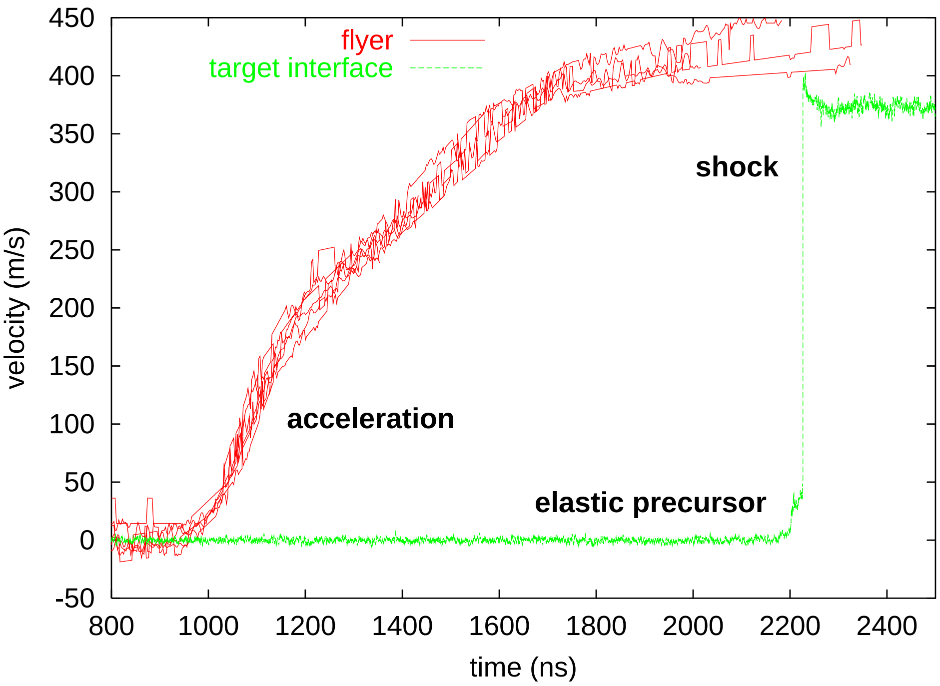


Example flyer impact data

Line VISAR record (streak camera) from window release experiment (shot 14124):

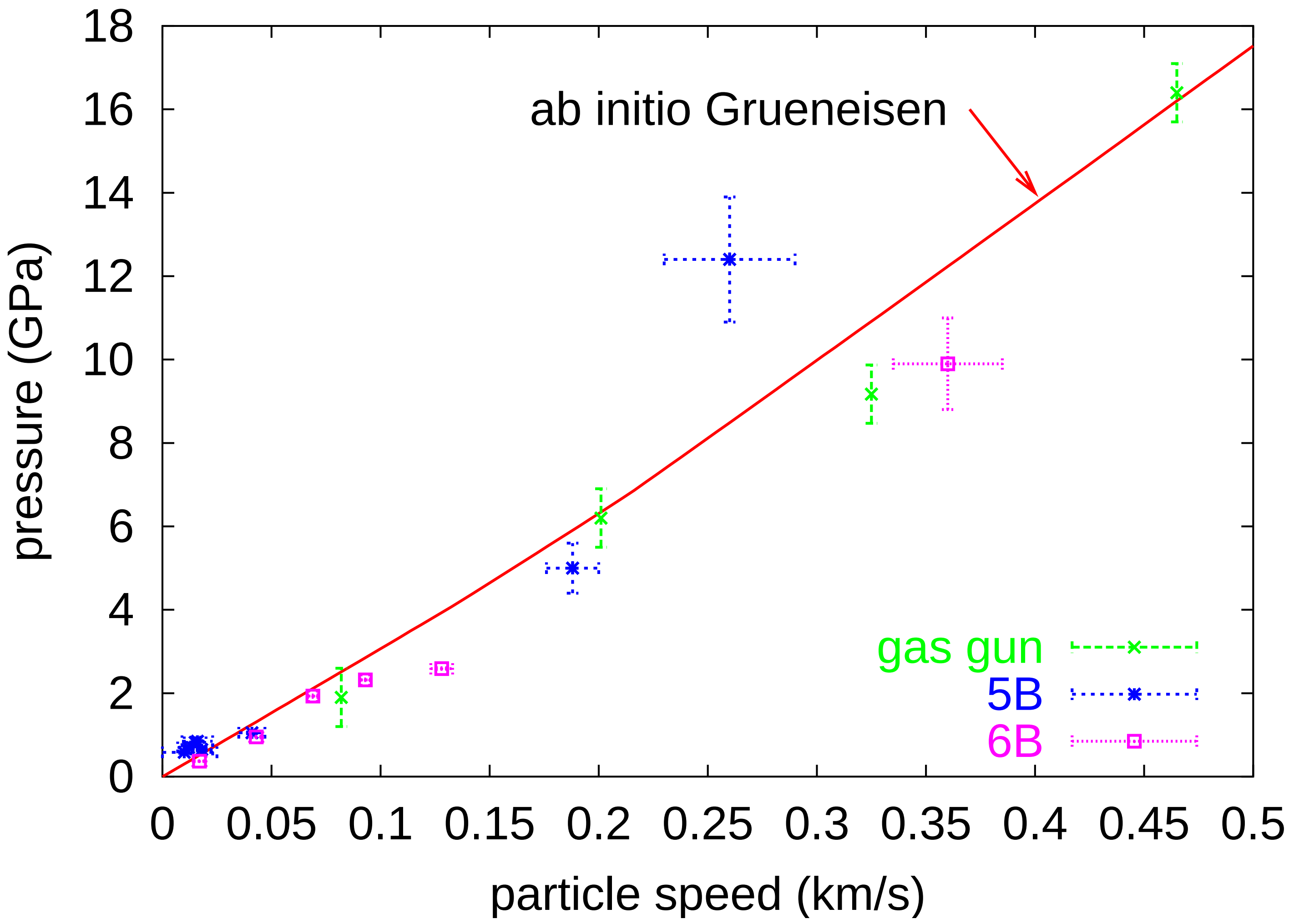


Reduced (otherwise unprocessed) velocity data:



Principal Hugoniot of NiTi

Theoretical EOS, laser flyer data (5B: 52.0 at % Ni; 6B: 54.2 at %), gas gun data (50.4 wt %) [Millett 02]:

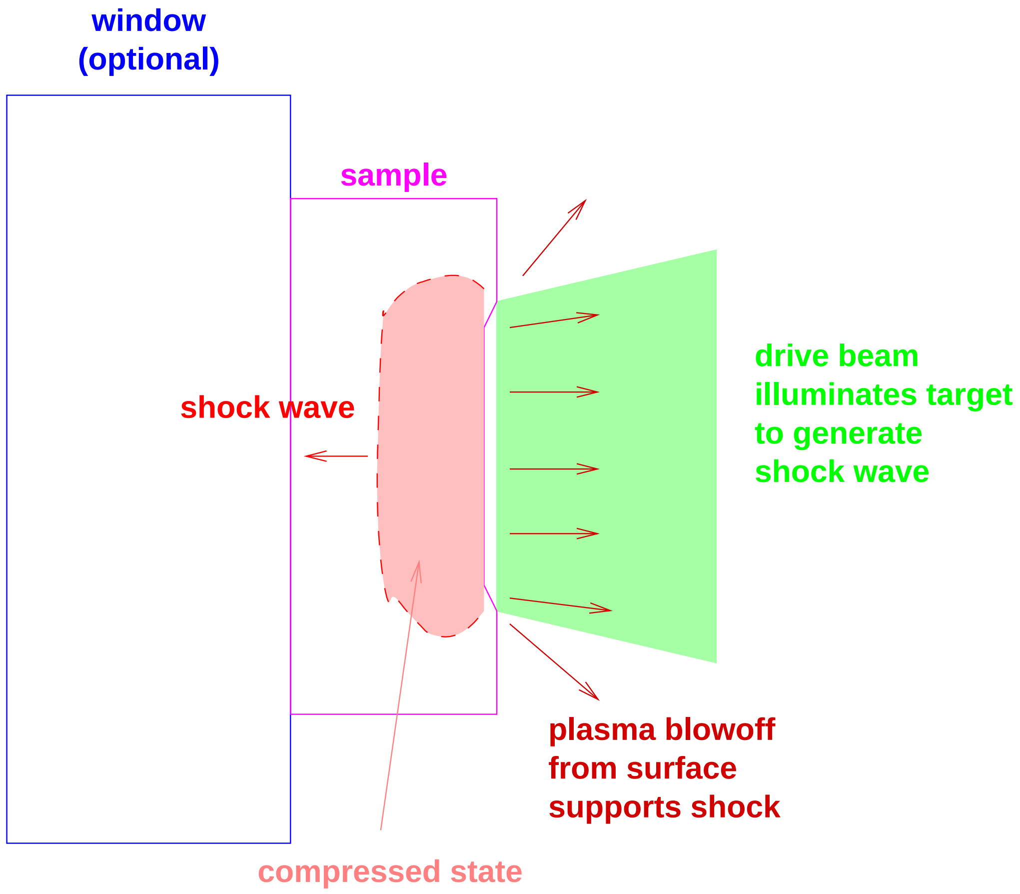


Flow stresses: apparently observed 0.35 and 0.95 GPa (uncertainty: 0.05 GPa) in different shots, bracketing quasistatic (0.5 GPa) and gas gun (0.8 GPa).

Spall stress from velocity pull−back: 1.5 GPa (5B) and 2.4 GPa (6B); uncertainty 0.2 GPa.

Direct−drive shock experiments

Used to load large numbers of samples efficiently, with recovery.

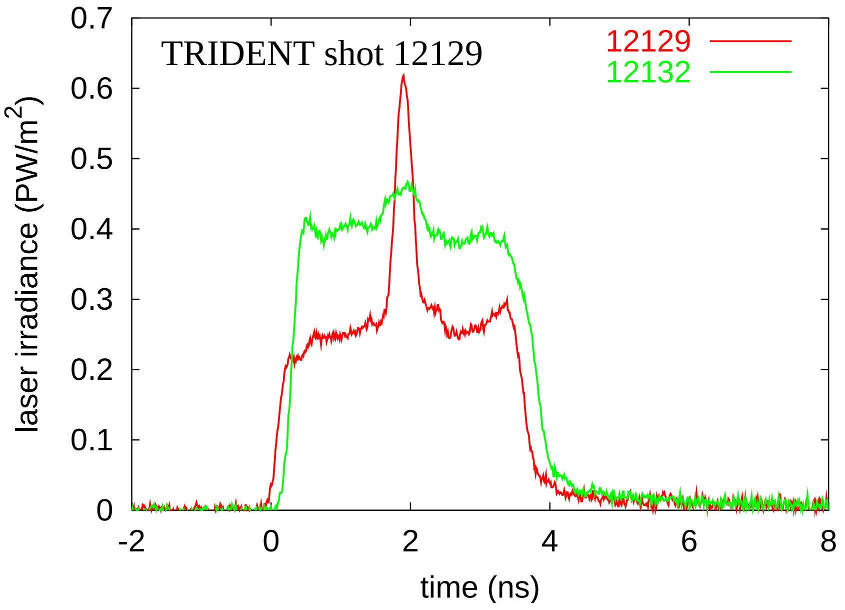


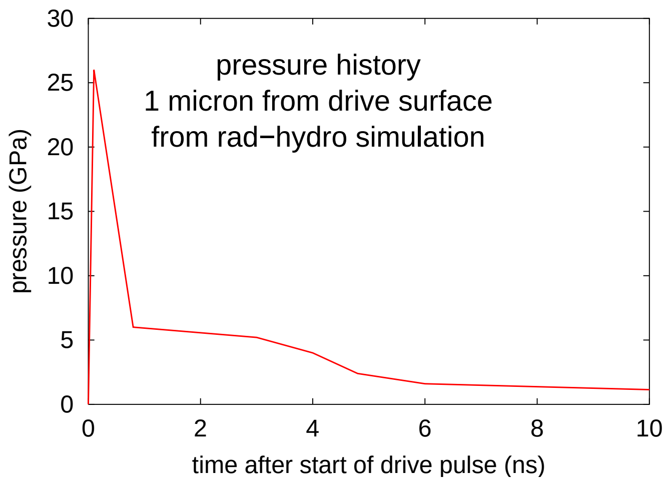
TRIDENT laser at 527 nm wavelength, pulses 0.2 to 3.5 ns long; pressures 1 to 20 GPa; up to 13 shots / day.
Re−usable target holder: minimized pre−shot assembly; sturdy construction helped for sample recovery.

Samples ~100 to 400 microns thick: decaying shock formed, exploring a wider range of states in each experiment.
Metallography was performed to investigate martensite/austenite formation and correlate with local loading history.
Results reported elsewhere.

Example result from direct drive shot

Laser can be used to induce exotic loading histories by temporal profiling of the irradiance, recorded on each shot. Sometimes, temporal shape can have unwanted features such as the spike on shot 12129.



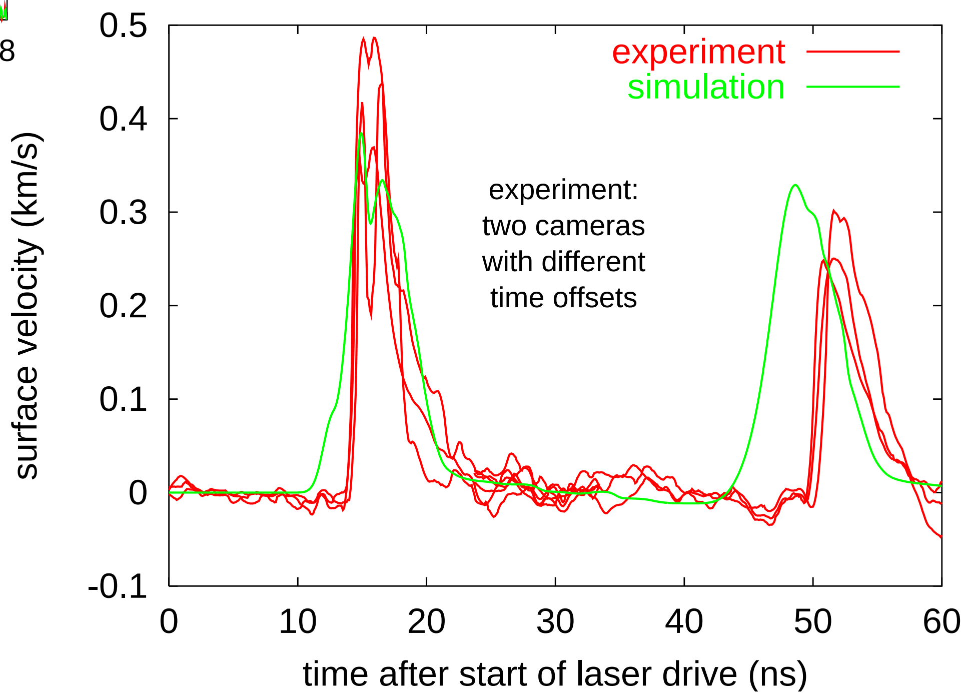


Radiation hydrodynamics simulations are used to predict loading history in sample, using measured irradiance history

Short timescale features have little effect on loading.

Surface velocimetry provides a check on accuracy of simulations and 1D−ness of drive.

NiTi: rad−hydro simulations need EOS and transport properties in regime of ablation plasma. We used "QEOS" model: not as successful as models for elements.



Conclusions

- Hugoniot EOS and dynamic strength of several NiTi alloys measured using laser-launched flyer impact experiments. EOS data matched, extended previous gas gun results using stress gauges; flow stresses bracketed value reported from static tests.
- Amplitude of precursor waves confirms previous identification of inflection near 3 GPa as onset of plastic flow.
- Ab initio quantum mechanics used to predict isotropic and uniaxial compression curves for NiTi in CsCl (B2) structure, used in turn to develop thermodynamically complete EOS and some elastic constants. Principal Hugoniot from EOS matched overall trend of the experimental Hugoniot states quite well. Elastic constants were consistent with the shear modulus from impact experiments.
- Prescription developed for simulating direct laser drive using radiation hydrodynamics; reasonable agreement obtained with laser ablation experiments.

Acknowledgements

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