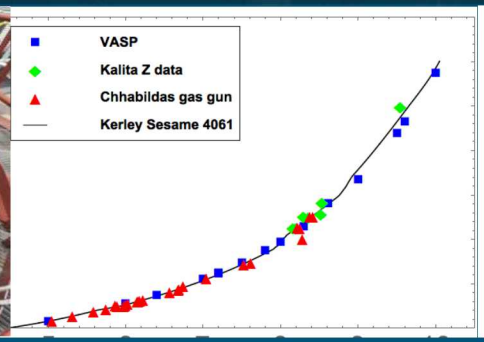
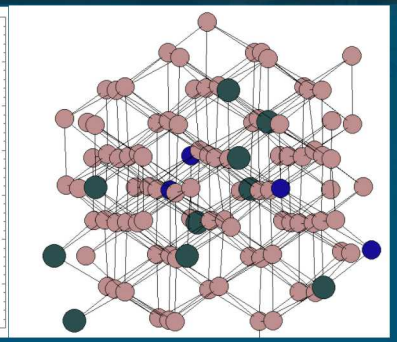
SAND2019-6702C

Computational and Experimental Hugoniot of Ti64 to 600 GPa





PRESENTED BY

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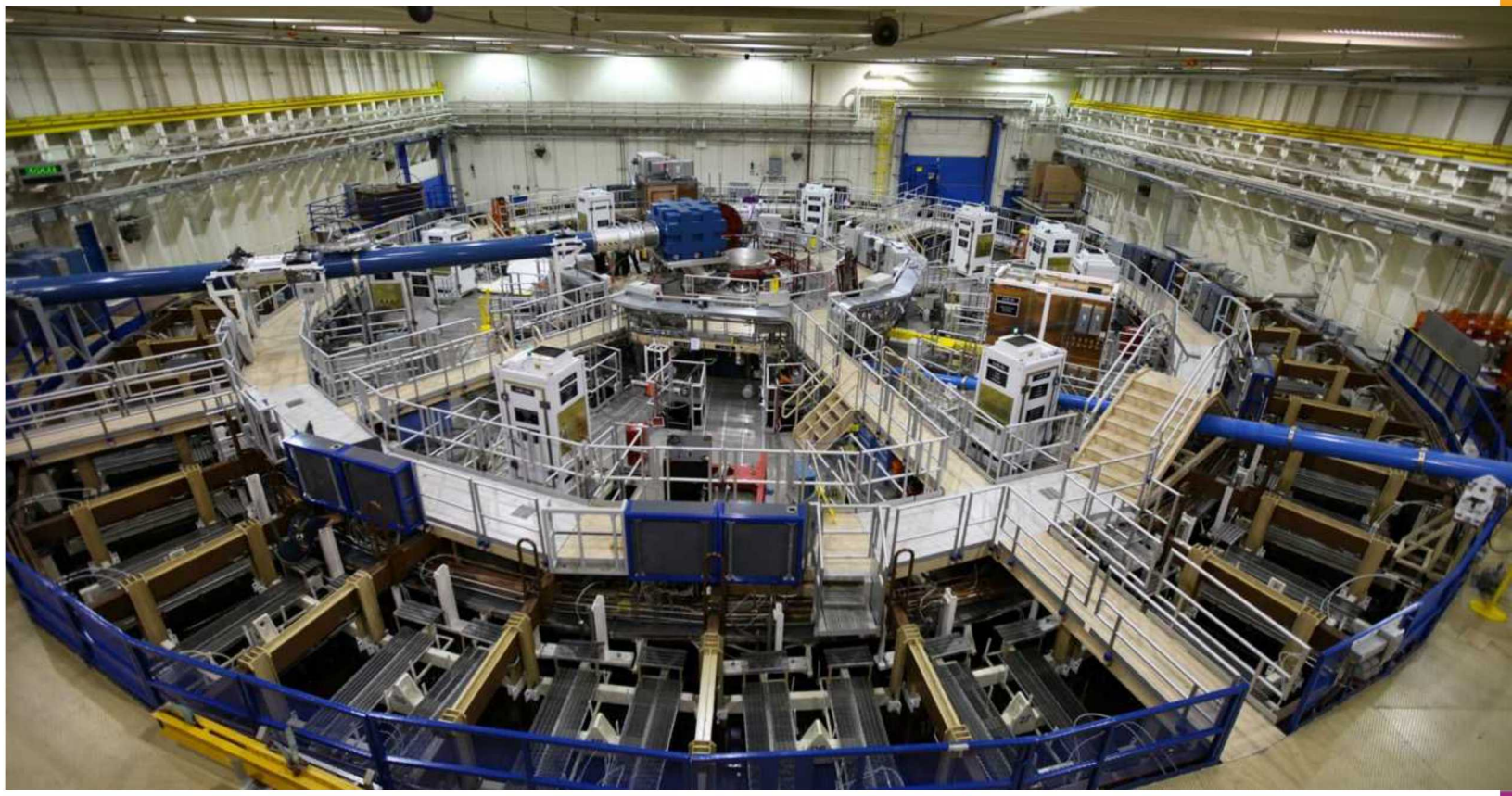
What is cool about Ti64?

- Ti64 = Ti_6Al_4V, is an alpha-beta titanium alloy Ti: 90 wt.%, Al: 6 wt.% V: 4 wt.%
- high strength-to-weight ratio and excellent corrosion resistance.
- diversified range of successful applications which demand high levels of reliable performance in surgery and medicine as well as in aerospace, automotive, chemical plant, power generation, oil and gas extraction, sports, and other major industries
- The EOS plays a key role in how a material changes volume and temperature during strong compression.
- We investigate the EOS of Ti64 using Sandia's Z machine and we use Density Functional Theory and the VASP code to predict and analyze the experiments.

Experiments on Sandia's Z machine

→ Why Z?: theory & data almost always diverge in previously unreachable regimes



Z: answer key physics questions

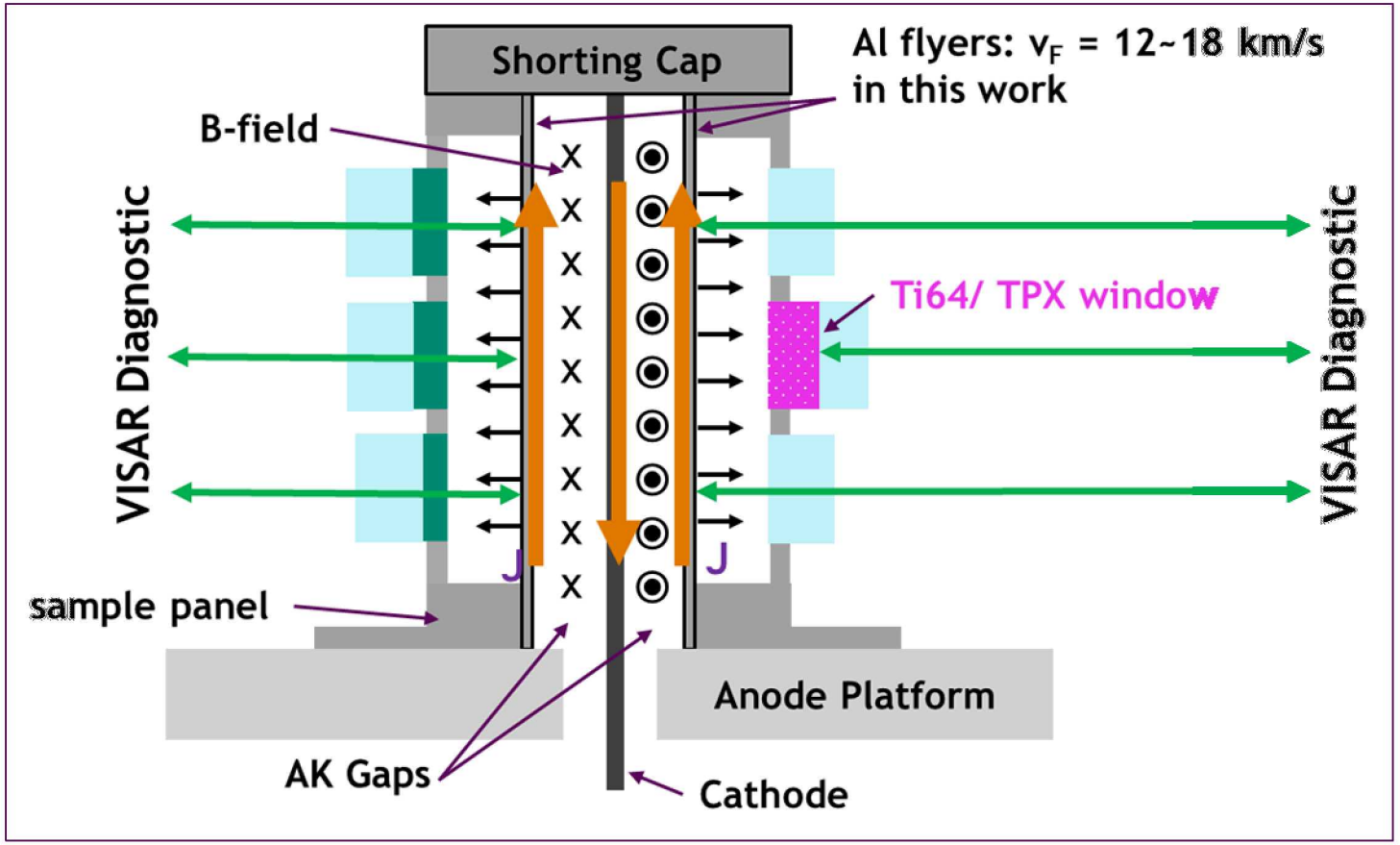
- Role of microstructure
- Kinetics and phase transitions
- Strength
- Transport properties
- Radiation shock

Z creates high pressures without directly heating materials:

- Long time scales (100-1200 ns) with control over the time history
- Large samples (cm): HED conditions in volumes ≫ sample grain dimensions

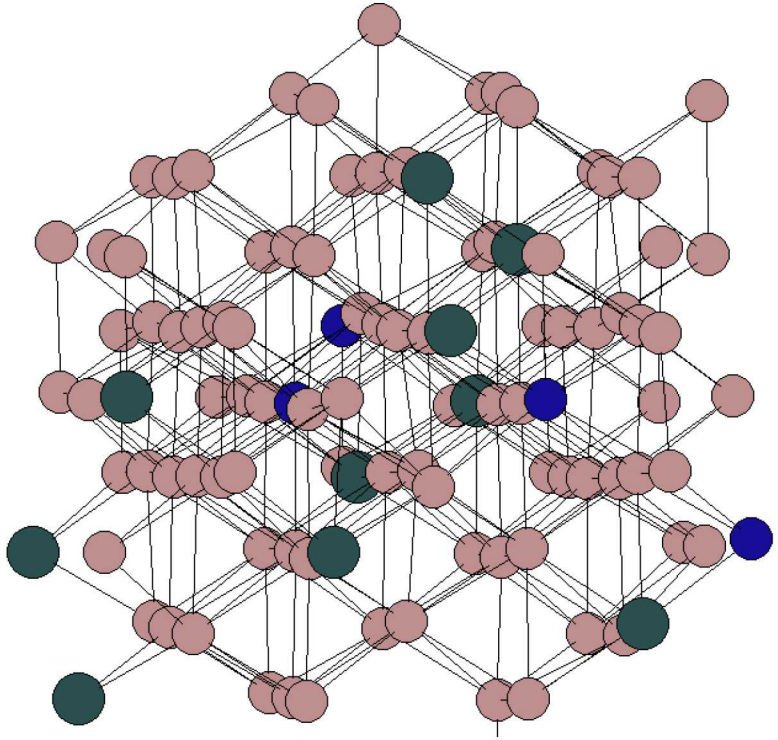
Experiments on Sandia's Z machine

- Opaque sample: Ti64 backed by transparent TPX window → VISAR records shock breakout time
- Transparent sample above and below → VISAR records impact time
- Impact and breakout time + sample thickness give shock velocity $\mathbf{U_S}$
- Monte Carlo impedance matching with the Al flyers gives the Ti64 particle velocity $\mathbf{u_P}$
- From data points in $\mathbf{U_S}$-$\mathbf{u_P}$ space we obtain data points in $\mathbf{P}$-$\boldsymbol{\rho}$ space



Use density functional theory (DFT) calculations to simulate Ti64

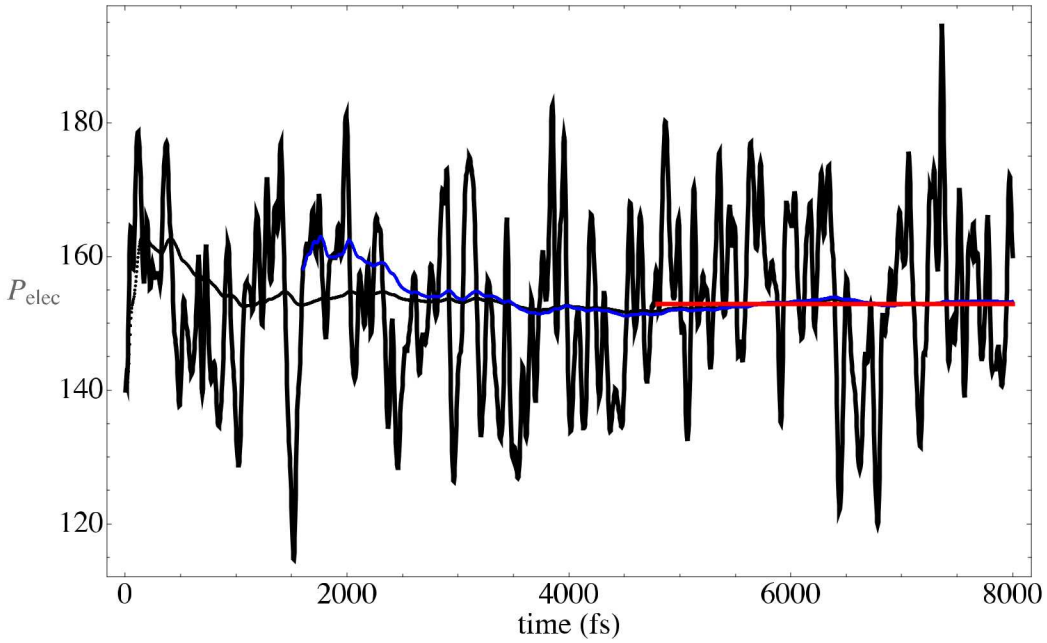
- **First-principles simulations DFT**
  - VASP – plane-wave code w PAW core-functions
  - Use of DFT codes simulating warm dense matter
    - *M. P. Desjarlais Phys. Rev. B **68**, 064204(2003)*
  - Great care in convergence
    - *A. E. Mattsson et. al. Modeling and Simulation in Material Science and Engineering **13**, R1 (2005)*
- **Assemble reference system**
  - Ti: 2 atom HCP structure
  - space group $P6_3/mmc$, axial ratio (c/a) ~ 1.58
  - 93 Titanium (brown), 11 Aluminum (green), 4 Vanadium (blue)
  - Random substitution of Al and V atoms into HCP lattice
  - PBE
  - Cutoff energy = 700 eV
- **Different random substitution patterns gave similar ambient pressures/energies**



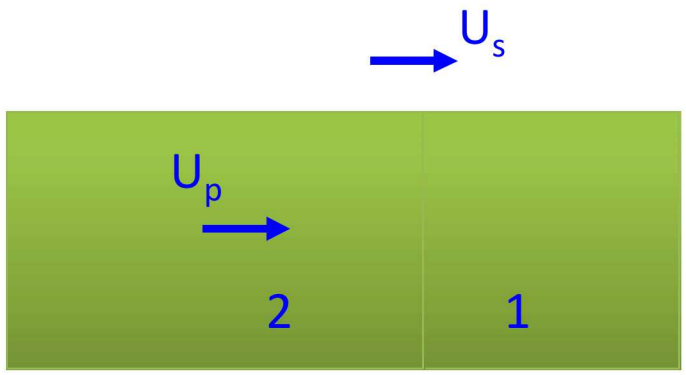
Quantum molecular dynamics (QMD) simulations give thermo-physical properties

Molecular dynamics simulations to converge to a pressure and energy

- **Typically tens of ps**
- **Simulation Size**
  - Larger number of atoms usually allow us to equilibrate in fewer time steps but take longer and more processors per time step
  - Higher probability of seeing stochastic events such as dissociation or melt at the correct density and temperature.
  - Smaller simulations become viable after melt.
- **Large oscillations in pressure and energy but the mean will of the block average < 1%.**
- **The mean pressure and energy are used to calculate the Hugoniot.**



Shock compression is a way to investigate thermo-physical properties of matter at extreme pressures



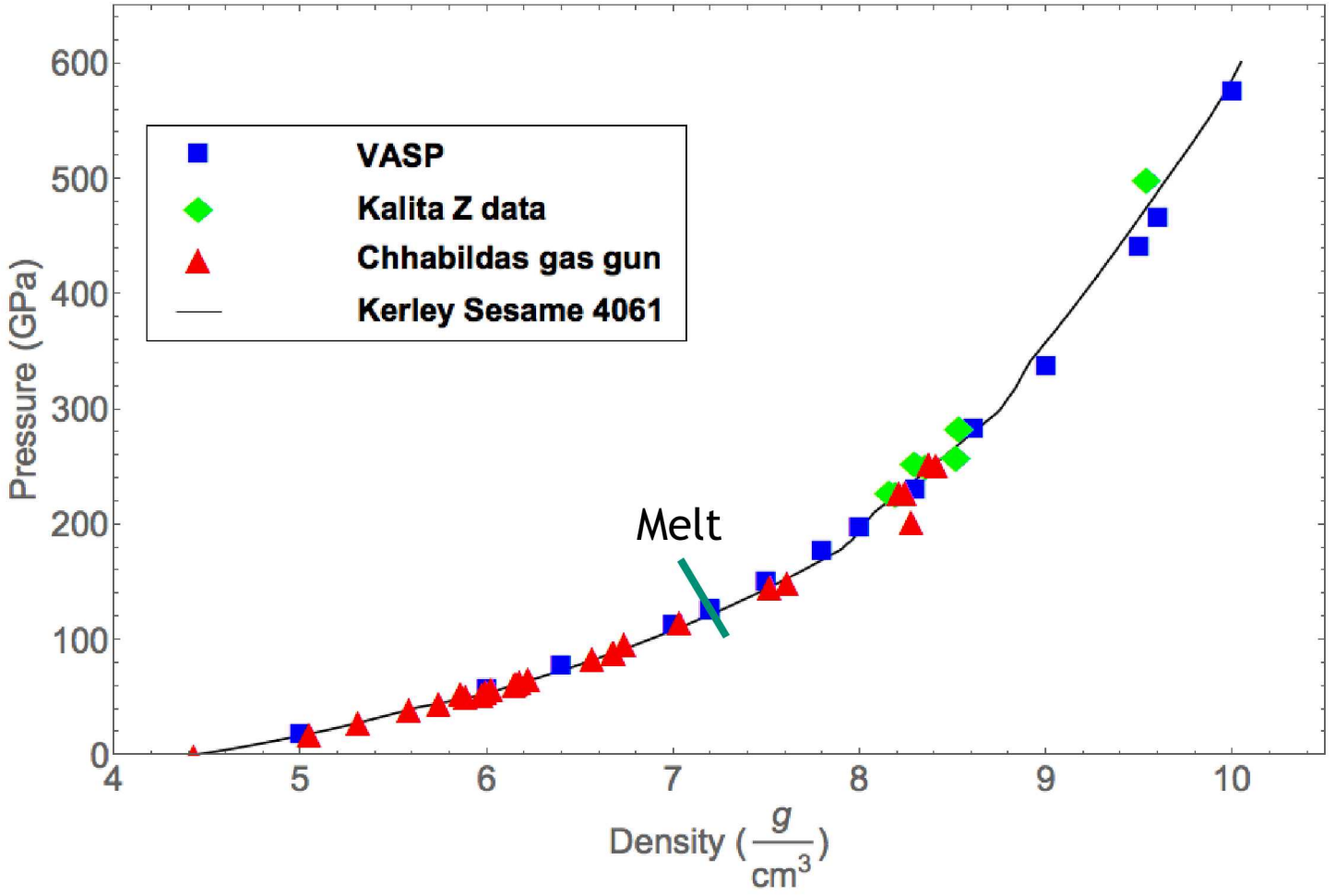
- *Conservation of mass, energy, and momentum* lead to the **Rankine-Hugoniot condition** for the initial (1) and final state (2)
  - E - internal energy
  - P - pressure
  - v – specific volume

$$2(E_2 - E_1) = (P_2 + P_1)(\upsilon_1 - \upsilon_2)$$

- *With high accuracy measure and/ or calculate thermo-physical properties*
- *First Principles Thermodynamics*

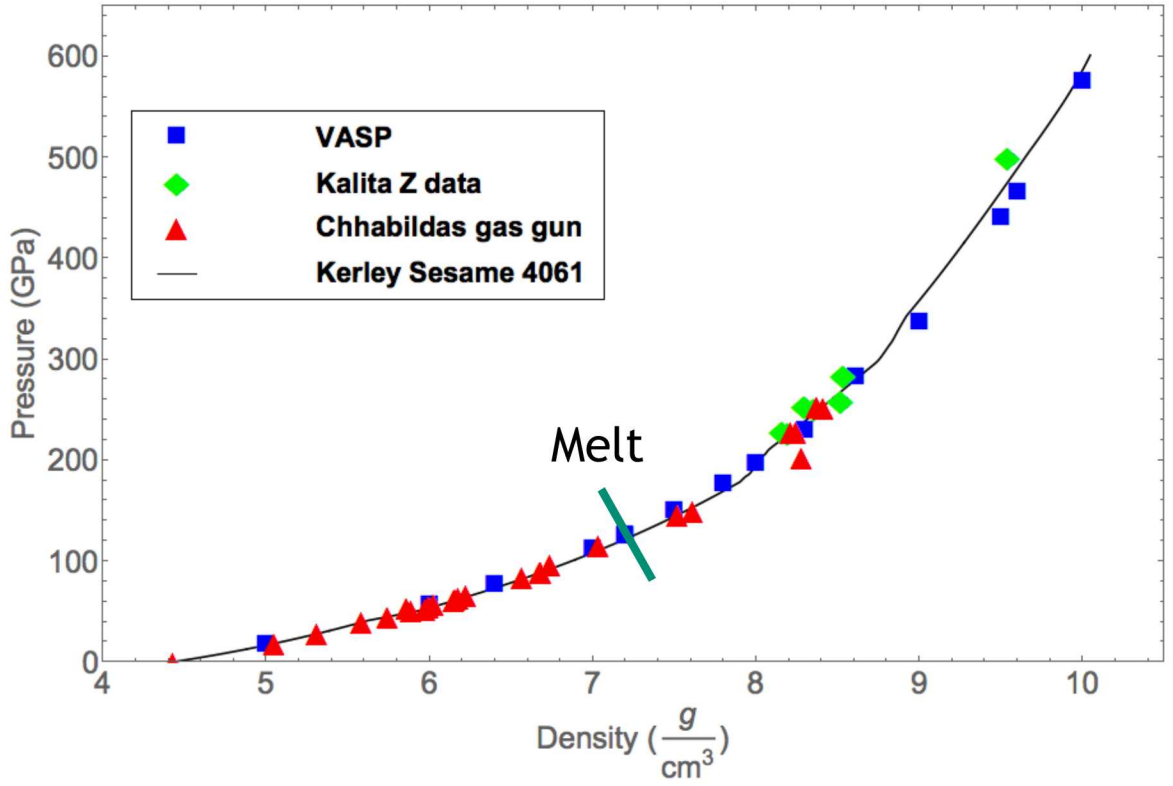
VASP QMD simulations vs. experimental data

- Hugoniot points calculated using the Erpenbeck method
- 2 bracketing simulations
- linear interpolation
- VASP has good agreement with experimental data
- Three stage gas gun data in agreement with lower pressure Z data
- Approximate melt between 7.0 and 7.2 g/cc
- 7.0g/cc temperature = 2550 K
- 7.2 g/cc temperature = 3025 K
- 7.5 g/cc temperature = 4150 K
- Does the melt transition go thru a molecular dissociation regime before becoming an atomic liquid?



Conclusions

- Random vanadium and aluminum substitution into titanium lattice
- Equilibrate simulation to steady state
- Erpenbeck method to calculate Hugoniot
- Good comparison to experimental data
- Ongoing work to determine if initial melt is atomic or molecular
- Both Kerley's equation of state and the new VASP calculations are in agreement with the experimental data up to 5 Mbar.
- Our results demonstrate that DFT can be used to predict high-pressure properties also of important alloys.



Acknowledgements

- Sandia National Laboratories Z-machine
- Sandia National Labs computing
- Los Alamos National Labs computing

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Experiments on Sandia's Z machine