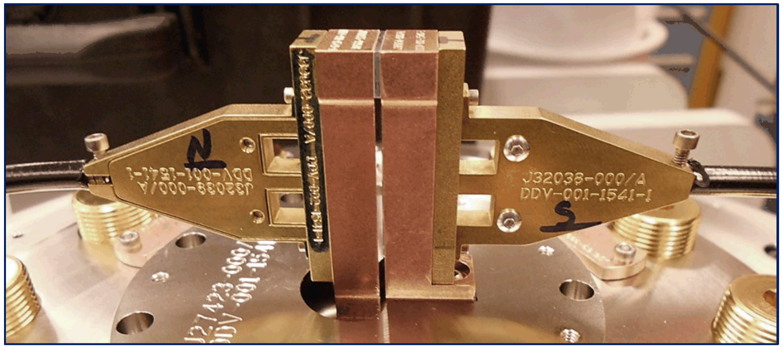
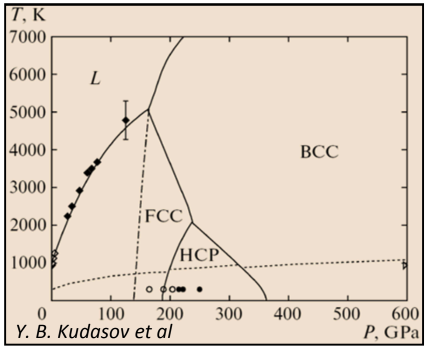
SAND2017-7147C





Phase Transitions in Aluminum Under Shockless Compression at the Z Machine

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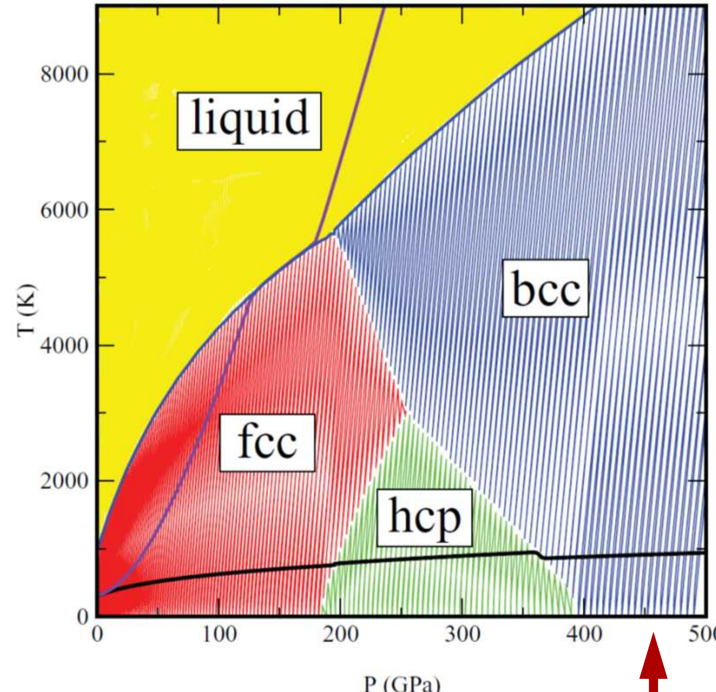
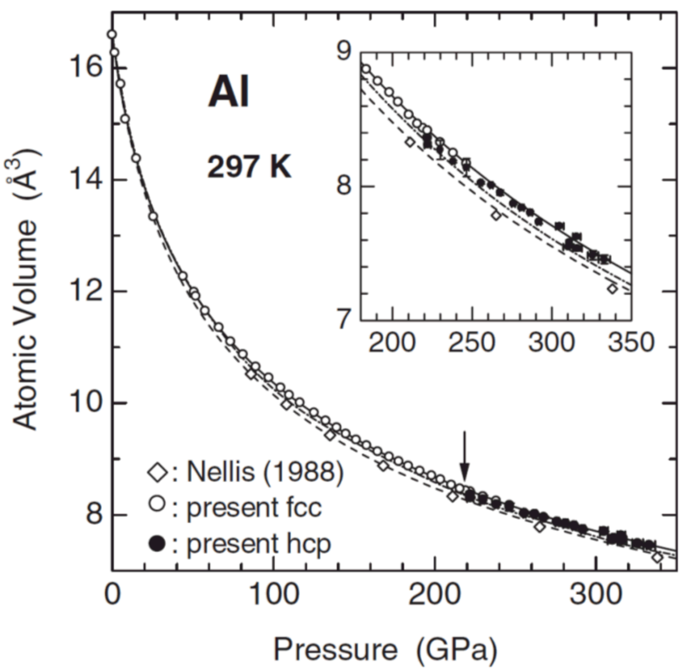
The existence of high-pressure solid structural phases in Al has long been theorized but only more recently observed

- Aluminum among simplest metals, ideal for testing theory
- Close-packed cubic structure and no 3*d* electron shell
- Used as standard in many dynamic compression experiments (guns, lasers, pulsed-power, …)
- Theory predicts FCC→HCP→BCC progression with pressure
- Only two known observations of non-ambient structure





Theory/Calculation:

AK McMahan & JA Moriarty, *Phys Rev B*, **27**, 3235 (1983)

GV Sin'ko & NA Smirnov, *J Phys Condens Matter* **14**, 6989 (2002)

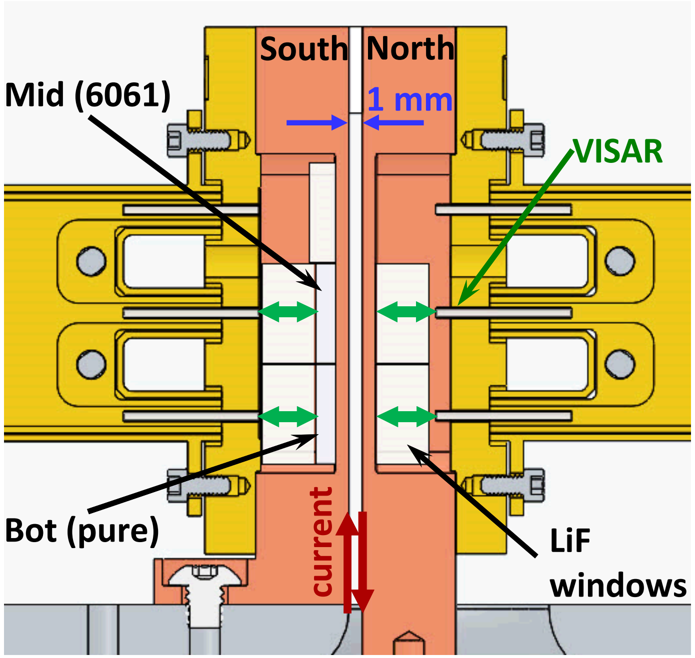
T Sjostrum et al, *Phys Rev B* **94**, 144101 (2016); **V6.00002**

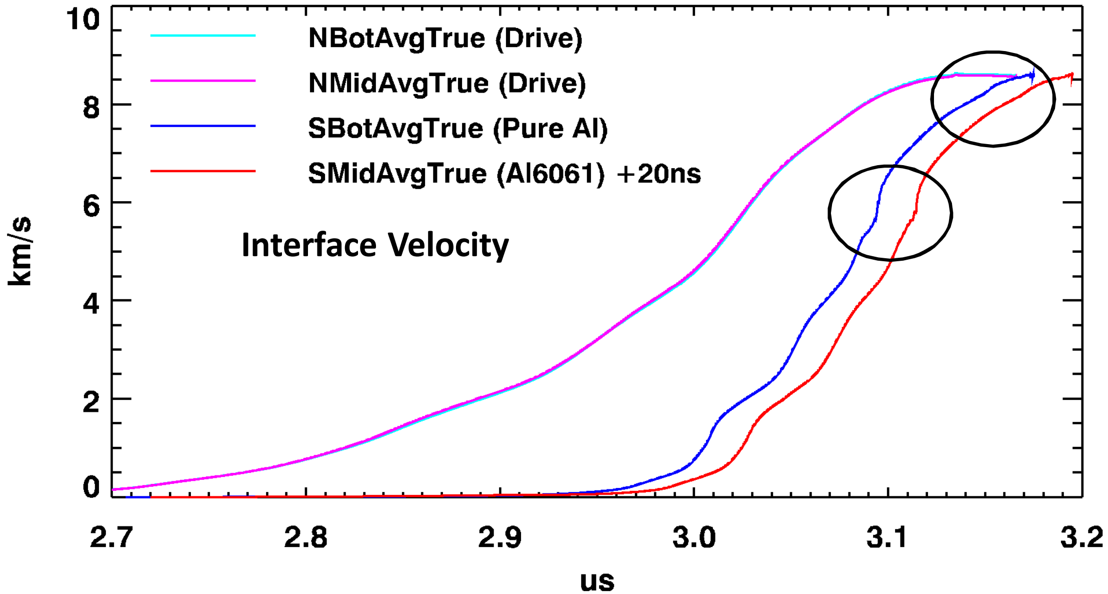
Experiment:

Y Akahama et al, *Phys Rev Lett* **96**, 045505 (2006)

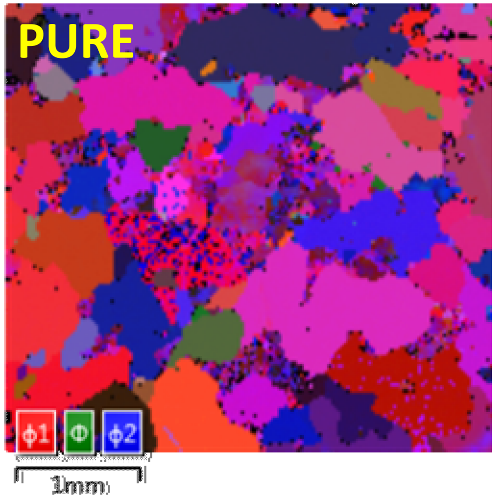
DN Polsin et al, **E7.00004** (to be submitted to *Phys Rev Lett*)

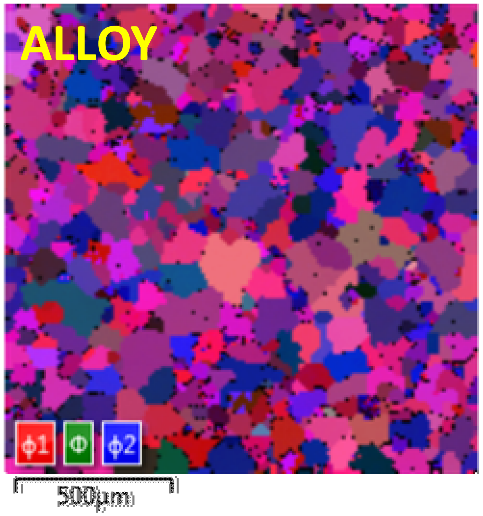
Experiment Z2878 shocklessly compressed pure and alloy aluminum samples to approximately 400 GPa





- Narrow, tapered, copper stripline load on Z
- Thin electrodes couple more P_{mag} to sample
- Square samples, 95-kV charge voltage on Z
- Pure Al had significantly larger grain size
- True velocity from VISAR correction using non-linear refractive index of LiF*



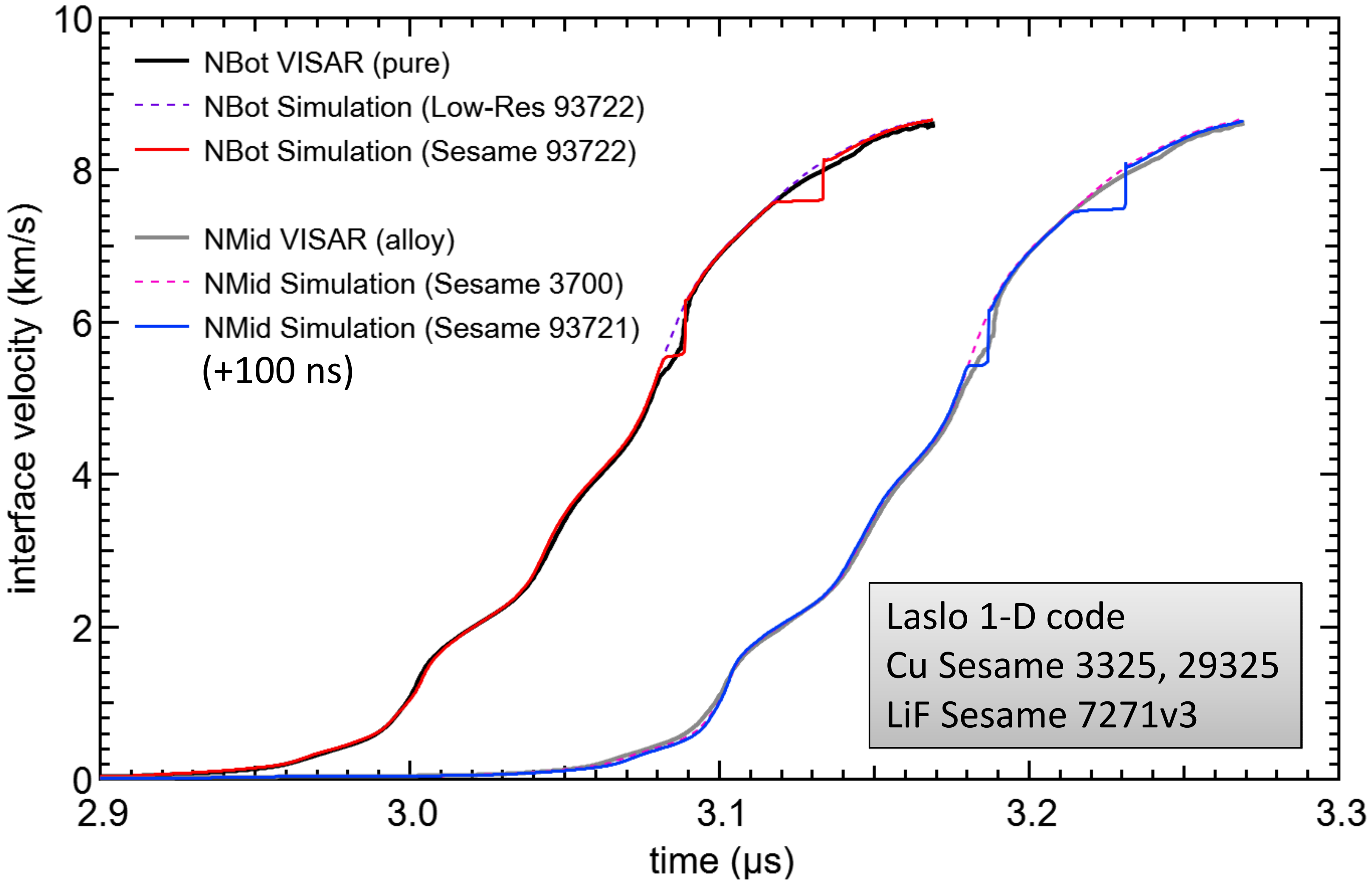


*J-P Davis et al, J Appl Phys **120**, 165901 (2016)

Velocity waveforms in good agreement with recent multi-phase tabular EOS from Los Alamos National Laboratory

Sesame 93722 = Al-1100 (≥ 99% pure)

Sesame 93721 = Al-6061 (≈96-98% pure) *T Sjostrum et al, Phys Rev B* ***94****, 144101 (2016)*



Extended Vinet EOS fit to recent LANL tabular EOS for each solid phase in order to simulate phase-transition kinetics

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- **Phase-transition kinetics model in Laslo 1-D hydrocode**
  - **only Mie-Gruneisen and Vinet individual-phase EOS available**
- Extended Vinet model uses 4-parameter cold curve + 2-parameter thermal EOS
- Fits are a reasonable approximation to tabular EOS (cold curves shown)

phase mass fractions

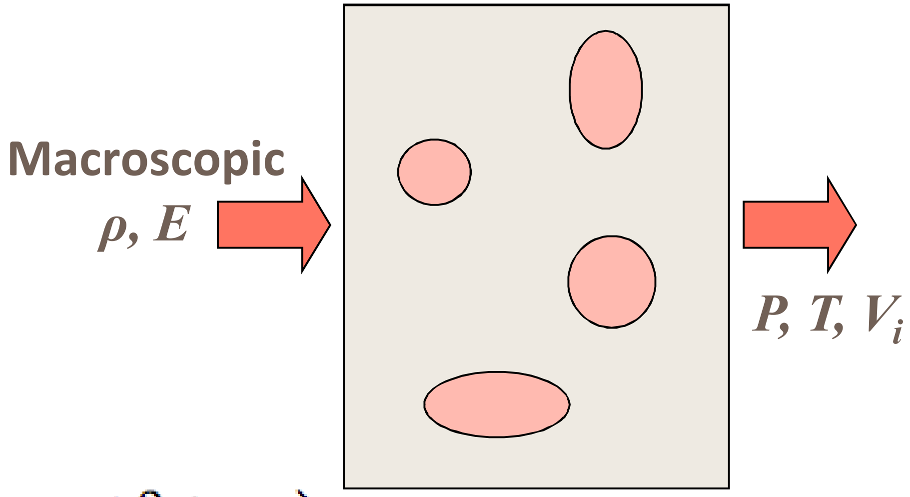
$$\sum_i \lambda_i = 1$$

transformation rates

$$\dot{\lambda}_i = \sum_j \left(\lambda_j R_{ji} - \lambda_i R_{ij}\right)$$

$$R_{ij} = \nu_{ij}\, \theta(G_i - G_j) \exp\left((G_i - G_j)^2 / B_{ij}\right)$$

Homogenized Continuum Model



PA Rigg et al, J Appl Phys ***106****, 123532 (2009)*

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$$P(V,T) = \frac{3B_0}{X^2} Z \exp(\eta_0 Z)\left(1 + \sum_{n=2}^{N} d_n Z^n\right) + \alpha_0 B_0 \left(T - T_{ref}\right)$$

$$X = \left(\frac{V}{V_0}\right)^{1/3}, \quad Z = (1 - X), \quad \eta_0 = \frac{3}{2}\left(B_0' - 1\right)$$

$$E(V,T) = 9\frac{B_0 V_0}{\eta_0^2}\left\{ f_0 - \exp(\eta_0 Z)\left[f_0 - \eta_0 Z \left(f_0 + \sum_{n=1}^{N} f_n Z^n \right)\right]\right\} - \alpha_0 B_0 V_0 \left(1 - X^3\right) T_{ref} + c_{V_0}\left(T - T_{ref}\right)$$

$$f_N = d_N, \quad f_n = d_n - \frac{n+2}{\eta_0} f_{n+1}, \quad d_0 = 1, \quad d_1 = 0$$

*P Vinet et al, J Phys Condens Matter **1**, 1941 (1989)*

Alegra User Manual (SAND2016-11878)

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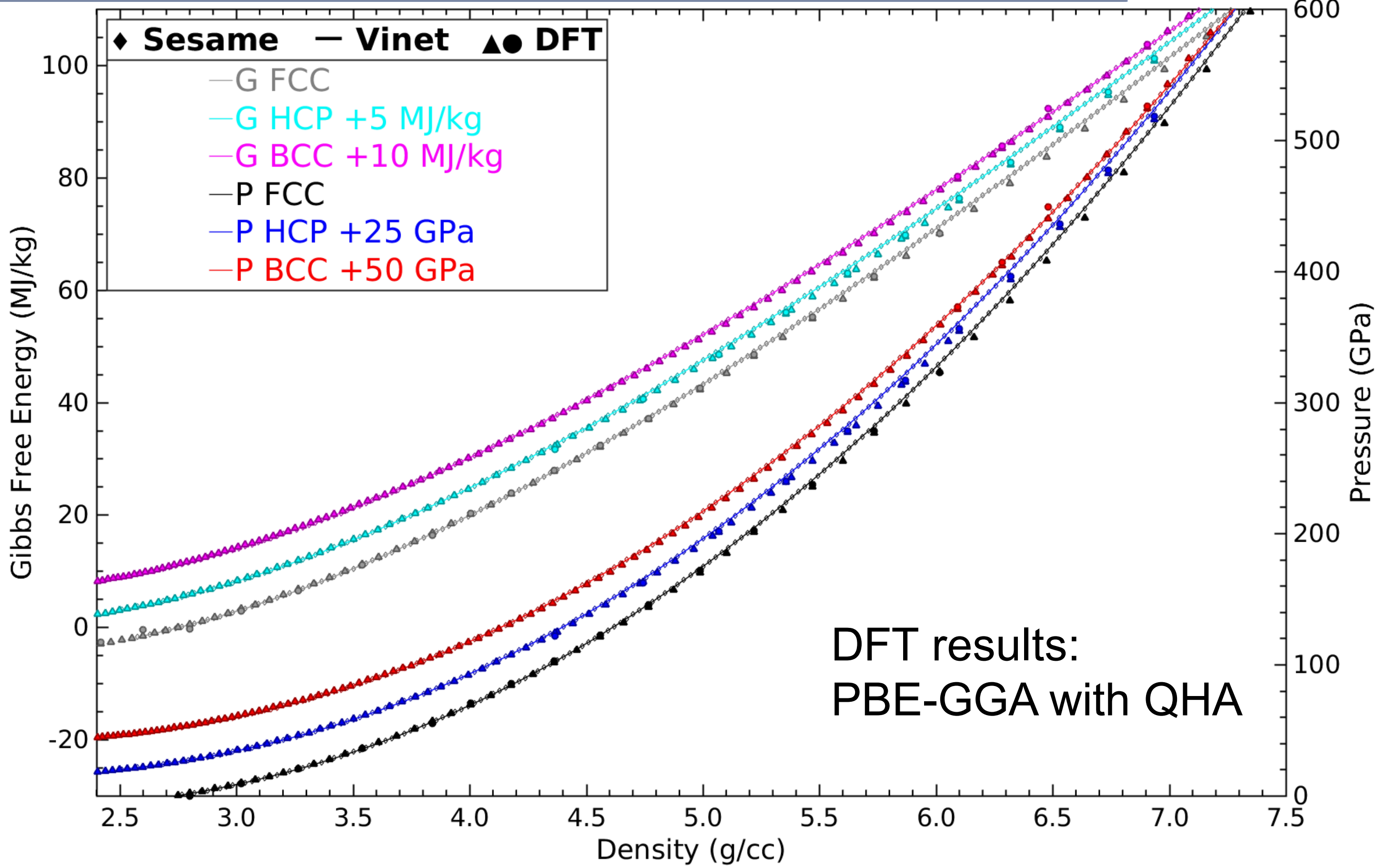

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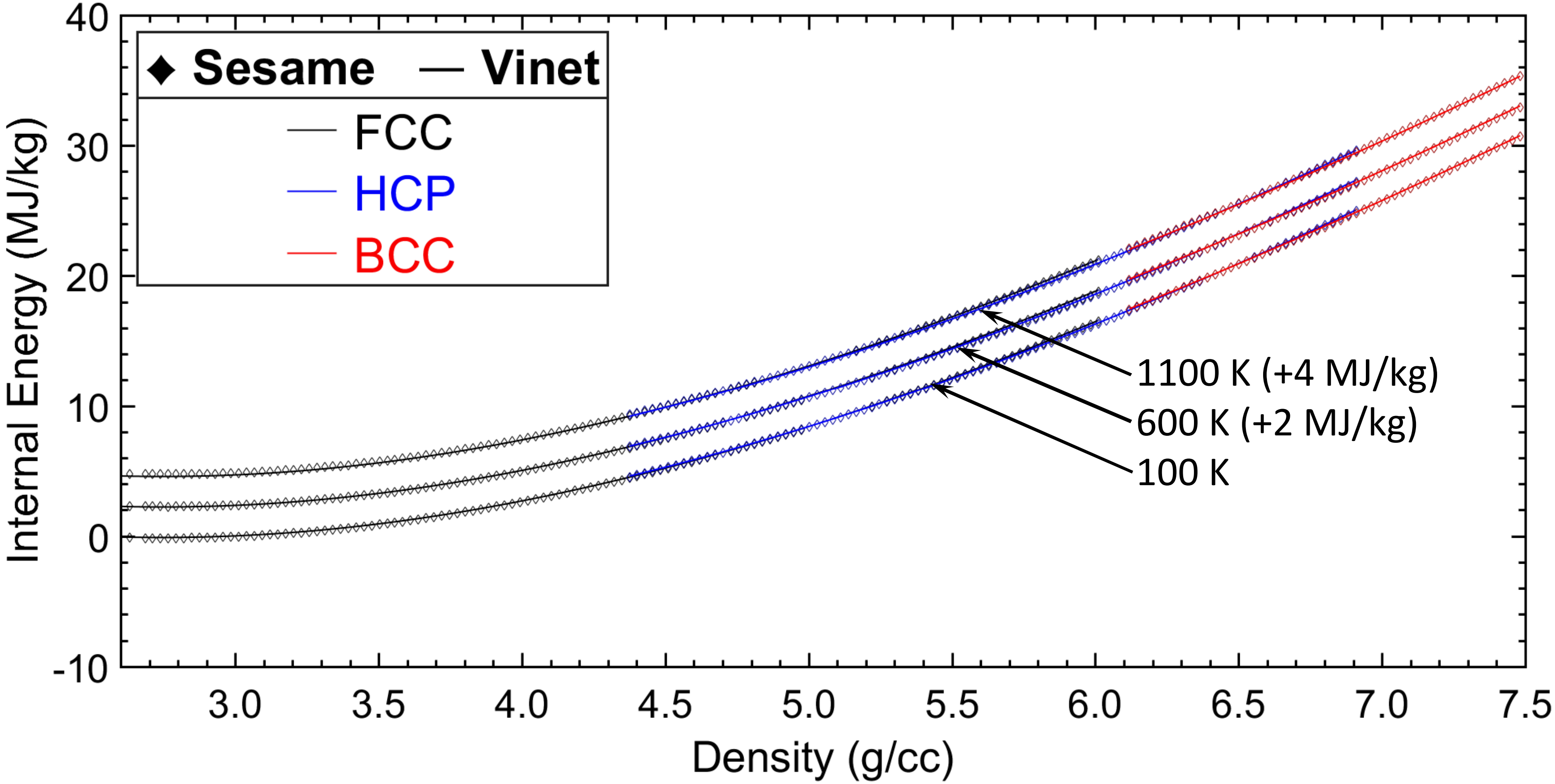
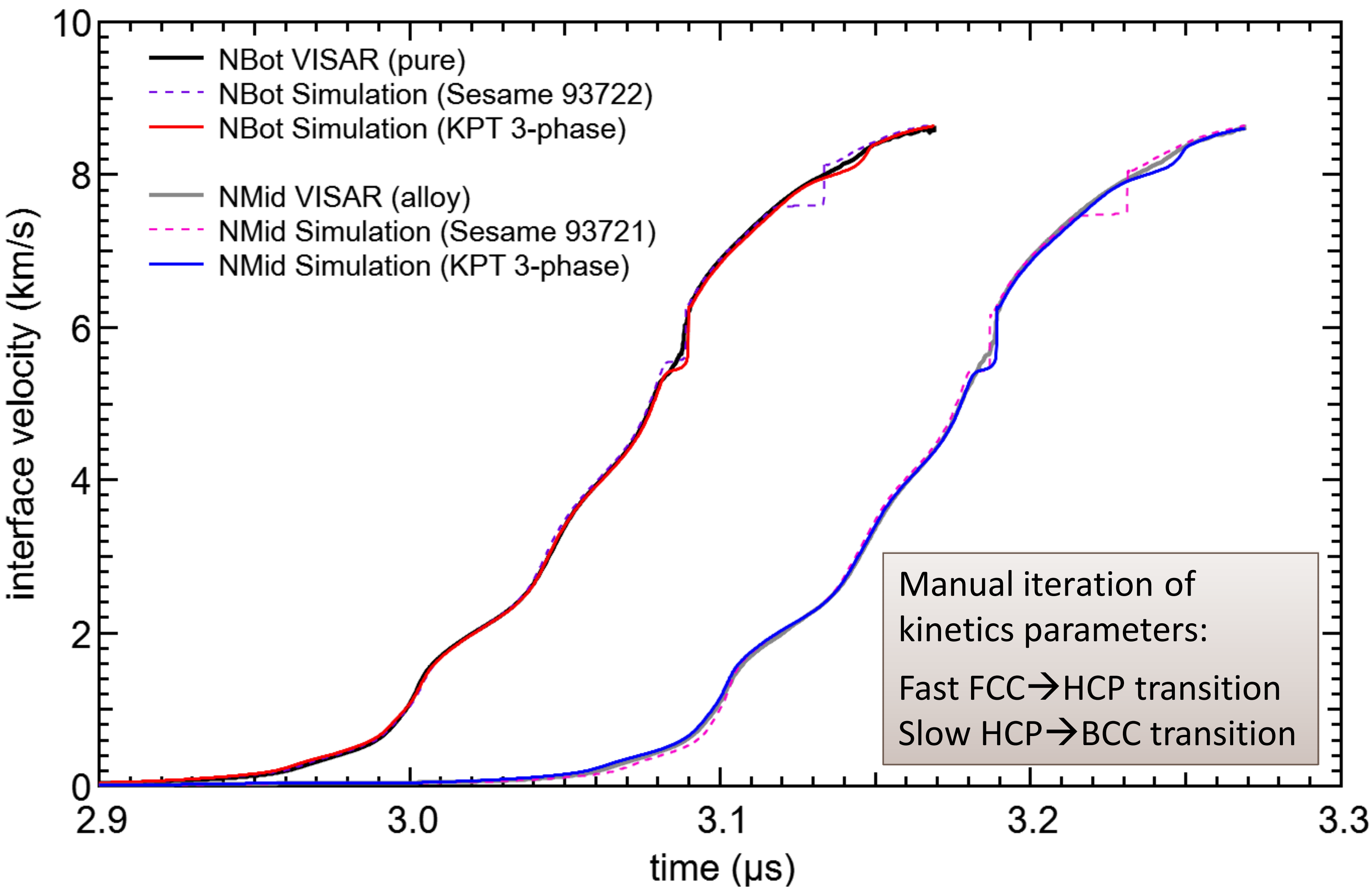
- **Fits are a reasonable approximation to tabular EOS (100/600/1100-K isotherms shown)**



Simulations using Kinetic Phase Transition (KPT) model and individual-phase Vinet fits improve agreement with data



Manual iteration of kinetics parameters:

Fast FCC→HCP transition
Slow HCP→BCC transition

Single-sample Iterative Lagrangian Analysis (ILA) of Z data captures post-transition HCP compressibility

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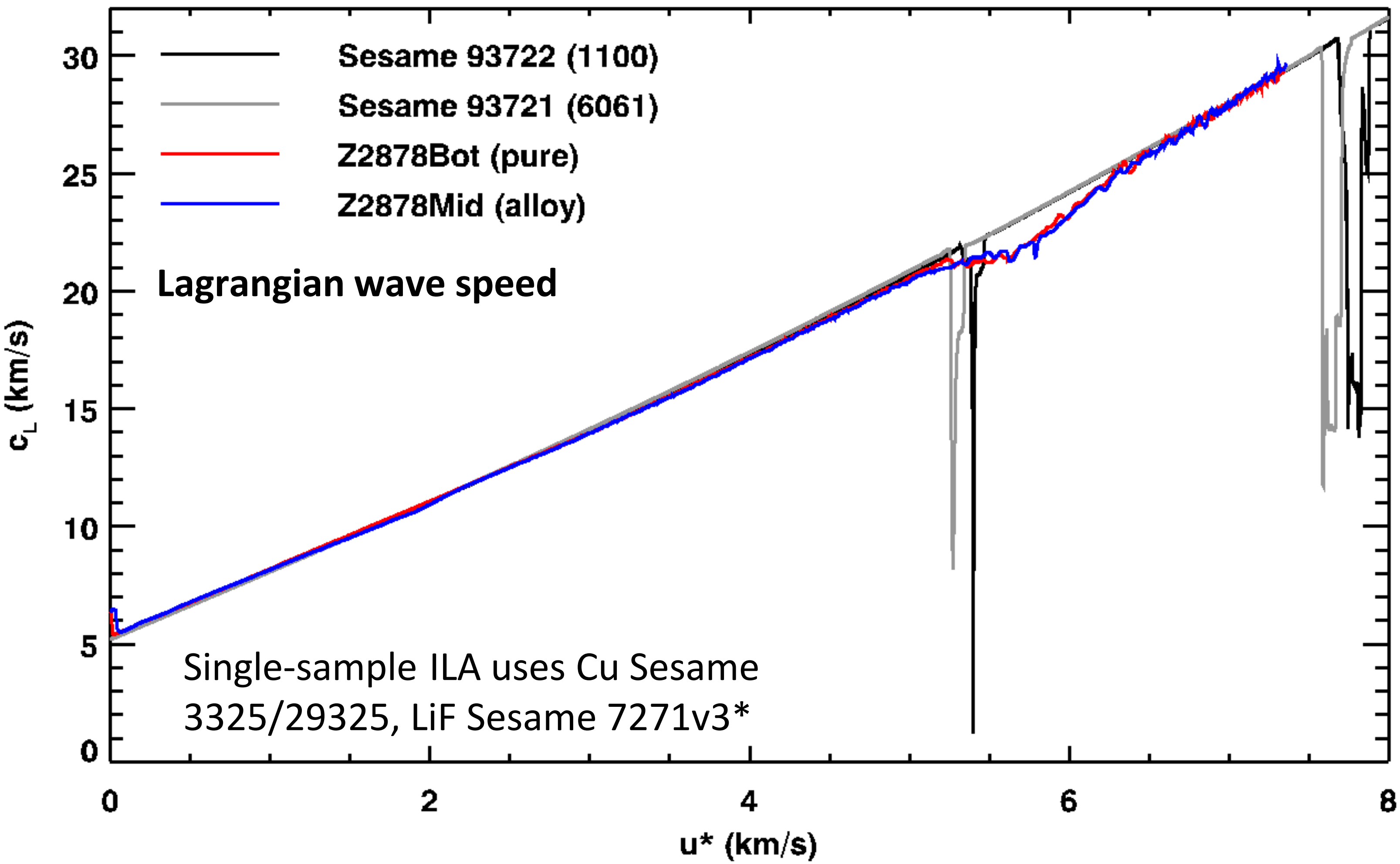

Conclusions and Future Work

- Velocimetry of pure and alloy aluminum shocklessly compressed to > 400 GPa
- Good agreement with new multi-phase tabular EOS
- Agreement improves using Kinetics Phase-Transition model with Vinet fit to tables
- Clear indication of fast FCC→HCP transition at expected stress of ~200 GPa
- Possible indication of slow/delayed HCP→BCC transition

Future Work:

- Automated calibration of kinetics parameters at fixed individual-phase EOS
- UQ to determine statistical significance of possible HCP→BCC velocity signature
- Implementation of tabular individual-phase EOS in Laslo KPT model
- More DFT calculations using QMC and anharmonic contributions
- Shock-ramp experiments to probe phase boundaries below and above triple-point