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Machine Learning in Atomistic Simulations for Additive Manufacturing Alloys

NIA Board of Directors Meeting

Vesselin Yamakov
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Collaborators

Edward Glaessgen – NASA/LaRC

Yuri Mishin – George Mason University (GMU)

Outline

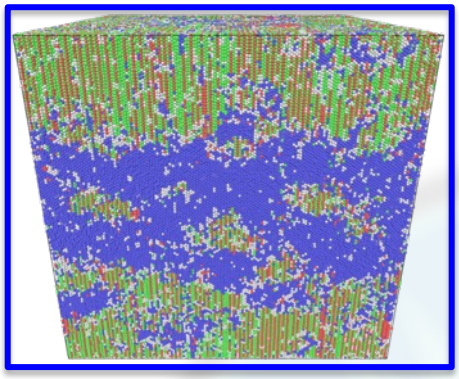
- Fundamental physics-based modeling of materials
- Atomistic simulations in additive manufacturing (AM)
- Machine learning in atomistic simulations
- Physically Informed Neural Network (PINN) interatomic potential
- Example for aluminum
- Computational implementation of PINN
- Conclusion

Fundamental Physics-Based Modeling of Materials

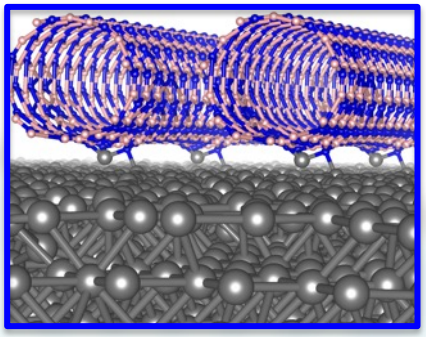
- Provides fundamental understanding of materials behavior
- Tailor materials properties to specific needs by composition and structural design
- Increases design space for advanced materials and enables new structural concepts

Atomistic Models

Phase transformation in CoNiAl SMA

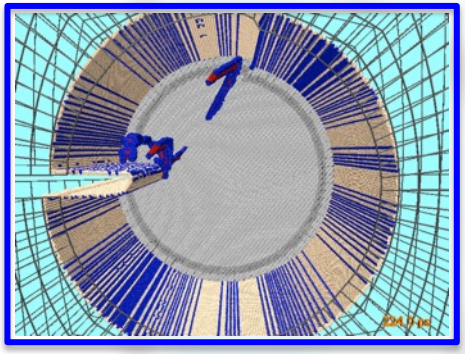


BNNT-Al metal matrix composite

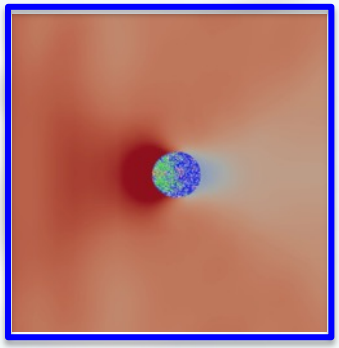


Multiscale Models

Crack tip plasticity in Al crystal



Pseudoelastic response of SMA particle under shock wave in Al matrix



Atomistic Simulations in Additive Manufacturing

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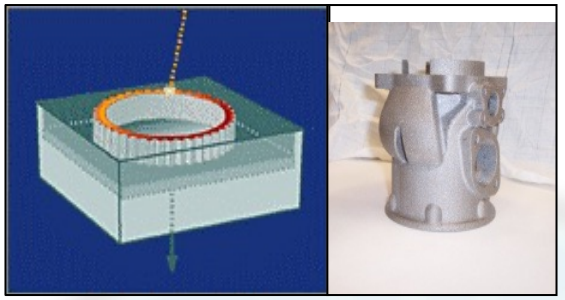
Role:

- Provides first-principles physics-based information on the highly dynamic AM processing during:
  - rapid heating and cooling (melt / solidification process)
  - strong thermal gradients (local heating)
  - high thermal stresses
- Complement other simulation methods at mesoscale by:
  - providing knowledge of microscopic mechanisms of key processes
  - obtaining material parameters not easily accessible experimentally

Objectives:

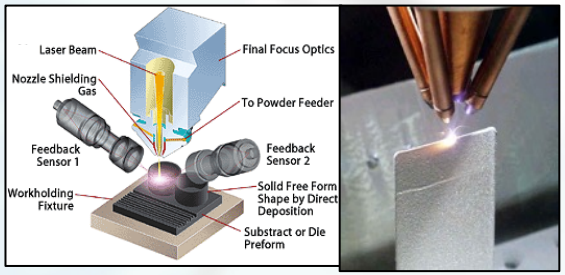
- Develop process parameter / microstructure relationships to guide process optimization
- Develop thermodynamics relationships to understand microstructure evolution and to guide design

Laser Sintering/E-beam Melting



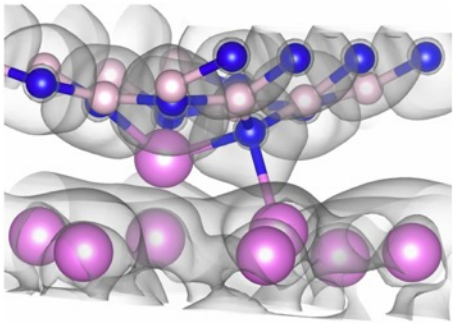
Electron Beam Freeform Fabrication

Laser Engineered Net Shaping



Machine Learning in Atomistic Simulations

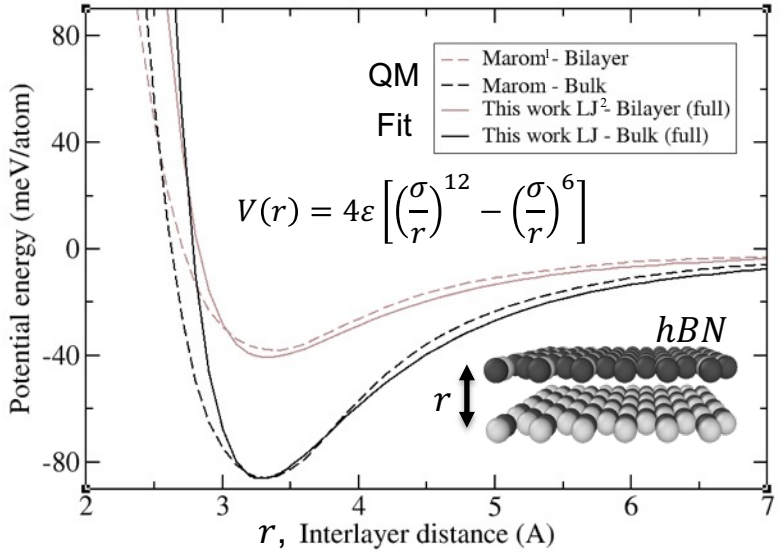
Atomic interactions governed by quantum mechanics (QM) are very complex and extremely difficult to calculate: cpu time $\sim N^{3\div 8}$



$$\hat{H}|\psi(t)\rangle = i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle$$

- Very accurate
- Generic to all known structures
- Very slow: cpu time ~N^{3-8}

Standard approach: replace the complex QM calculations with a simplified expression with empirically fitted parameters



- Very fast: ~10^{12} atoms
- Inaccurate
- Non-transferable (unique for each material)
- Difficult to create (expensive)

[1]N. Marom et al., Phys. Rev. Lett. 105 (2010) 046801.
[2]V. Yamakov et al., Comp. Mat. Sci. 135 (2017) 29.

New approach is needed

Physically Informed Neural Network (PINN) Interatomic Potential

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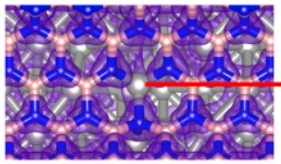
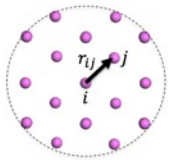
The Universal Approximation Theorem: a neural network (NN) can approximate any f(x)

NN universality



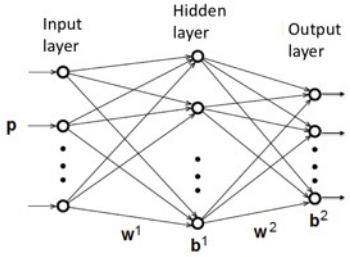
Material



Atomic environment

$$\begin{pmatrix} G_1 \\ G_2 \\ \vdots \\ G_n \end{pmatrix}$$

Structure coefficients



Neural Network

Contains the "knowledge" of the QM calculations

$$\begin{pmatrix} A_i \\ \alpha_{ij} \\ B_i \\ \beta_{ij} \\ \vdots \end{pmatrix}$$

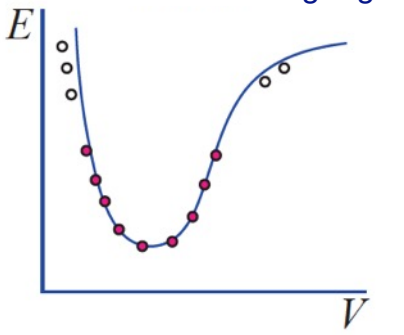
NN predicted parameters

$$\frac{1}{2}\sum_{j\neq i}\left[e^{A_i-\alpha_{ij}r_{ij}} - S_{ij}b_{ij}e^{B_i-\beta_{ij}r_{ij}}\right]f_c(r_{ij}) = E_i$$

NN parameterized potential energy function

Retains the physics of the atomic interactions

Improves transferability outside the training region

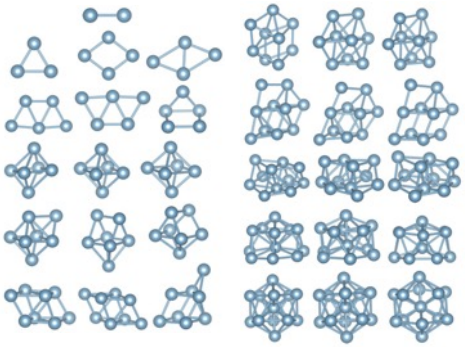


QM is replaced by a trained NN

Implementation of PINN

Training Stage

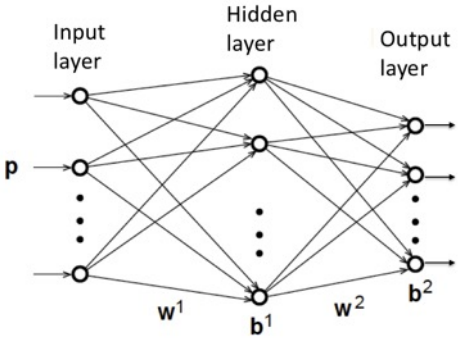
Use QM to calculate a large set of atomic structures



$$\begin{pmatrix} E_1 \\ E_2 \\ \vdots \\ E_n \end{pmatrix}$$

$$\hat{H}|\psi(t)\rangle = i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle$$

Train NN against $\{w^1, b^1, w^2, b^2, \dots\}$ to minimize the objective function, ε



$$\begin{pmatrix} A_i \\ \alpha_{ij} \\ B_i \\ \beta_{ij} \\ \vdots \end{pmatrix} \rightarrow f(A_i, \dots, r_{ij}) = E_i$$

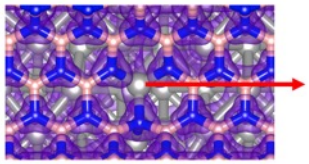
$$\varepsilon = \sum_n (\tilde{E}_i - E_i)^2$$

Objective function:

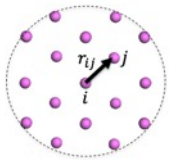
$\varepsilon \rightarrow 0$

Inference Stage

Fixed $\{w^1, b^1, w^2, b^2, \dots\}$ as trained



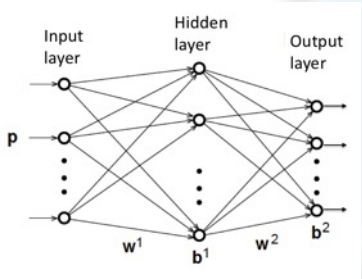
Material



Atomic environment

$$\begin{pmatrix} G_1 \\ G_2 \\ \vdots \\ G_n \end{pmatrix}$$

Structure coefficients

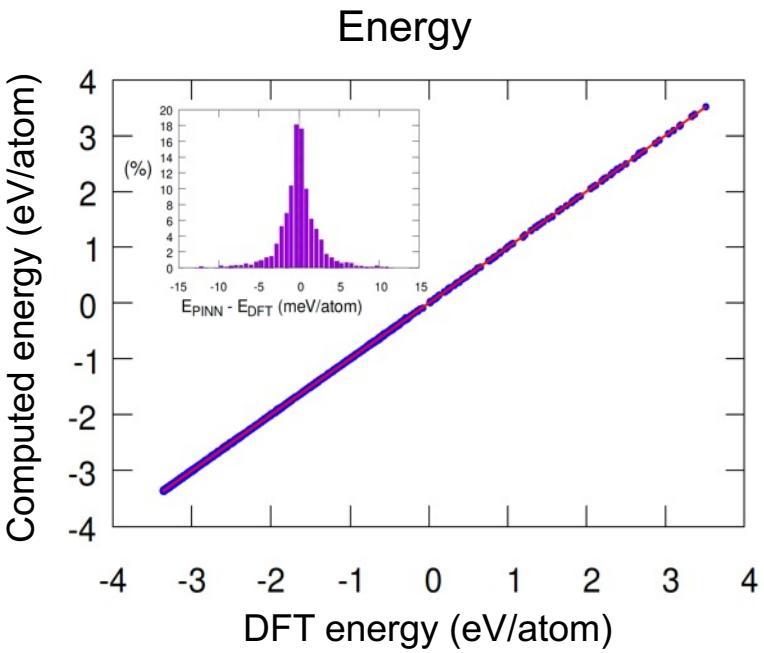


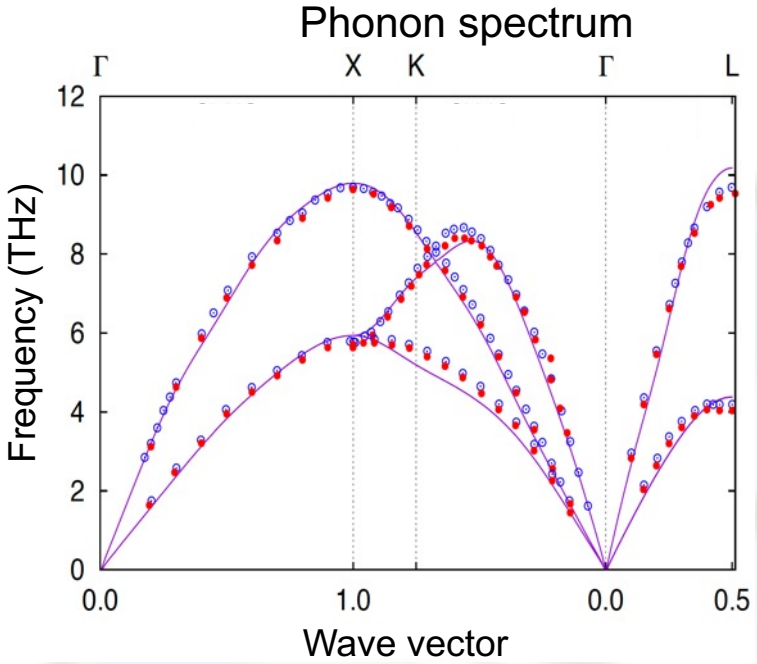
$$\begin{pmatrix} A_i \\ \alpha_{ij} \\ B_i \\ \beta_{ij} \\ \vdots \end{pmatrix} \rightarrow \frac{1}{2}\sum_{j\neq i}\left[e^{A_i-\alpha_{ij}r_{ij}} - S_{ij}b_{ij}e^{B_i-\beta_{ij}r_{ij}}\right]f_c(r_{ij}) = E_i$$

Approximate E_i of atom (i):

Retains the accuracy of QM while gaining in speed: cpu time ~N

Example for Aluminum: Crystalline Phase





DFT – Density Functional Theory calculations

NN architecture: 40x16x16x8 -> 1064 fitting coefficients

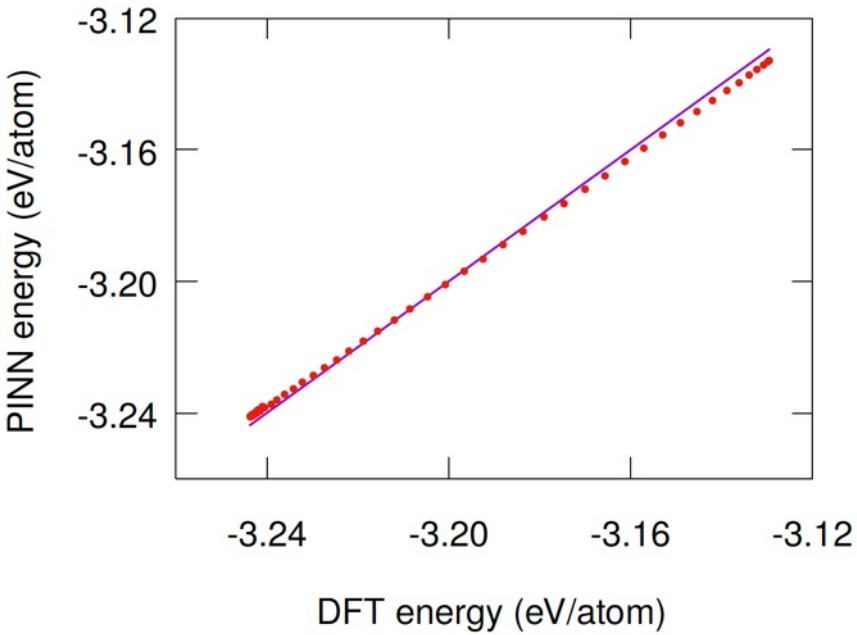
Training set: 36,490 supercells of 2 to 79 atoms

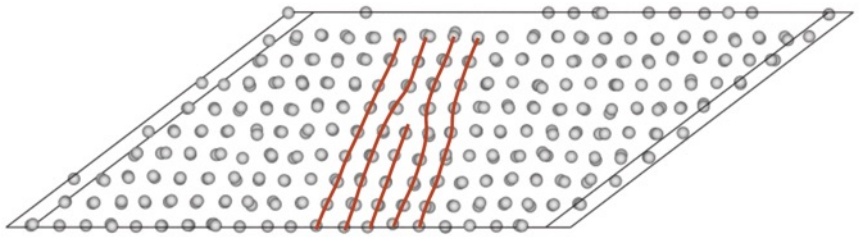
G. P. Purja Pun et al., *Physical Review Materials*, 4 (2020) 113807.

Excellent fit to DFT (QM) calculations

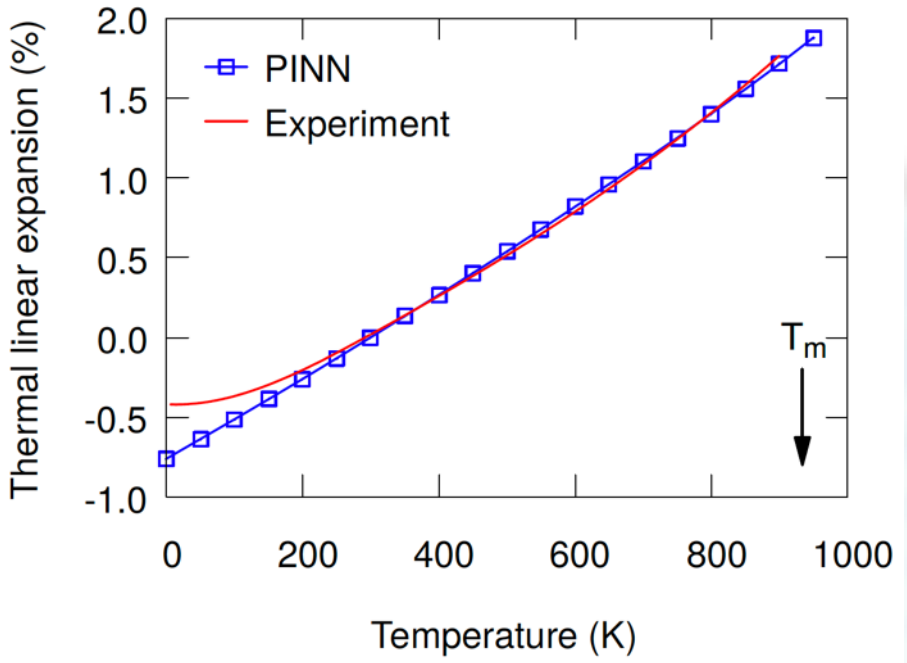
Example for Aluminum: Defect Structures

Edge dislocation





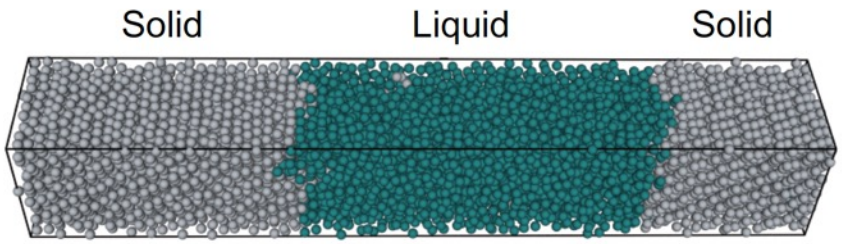
Thermal expansion

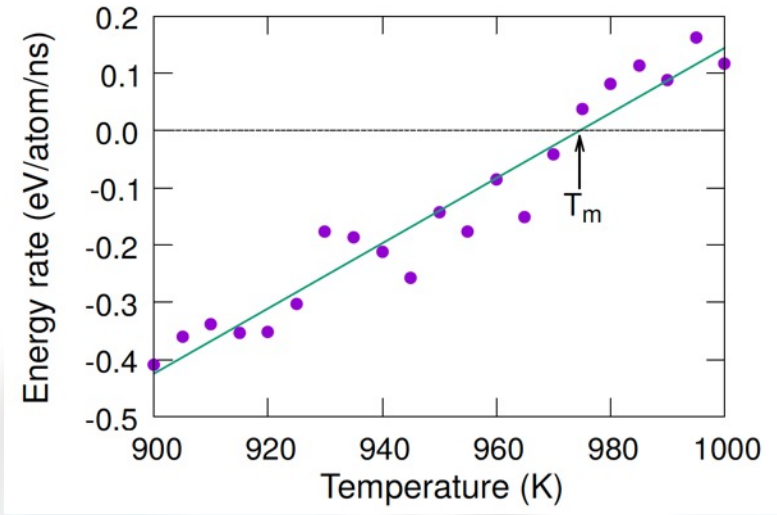


Excellent agreement with defect structures and thermal expansion

Example for Aluminum: Melt Properties

Melting temperature





$$T_{m\,(NN)} = 975\ K$$

$$T_{m\,(experiment)} = 933\ K$$

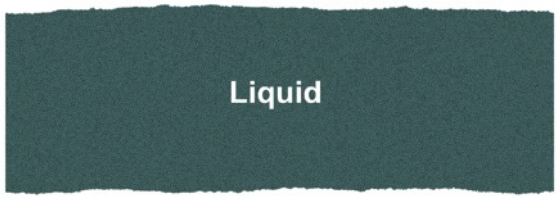
Reasonably good prediction of the melting temperature

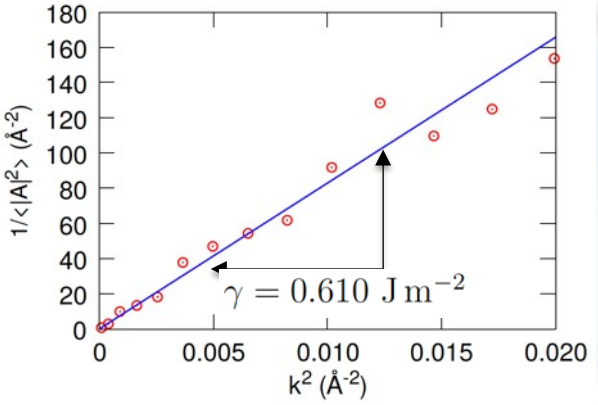
Example for Aluminum: Melt Properties

Surface and liquid-solid interface energies

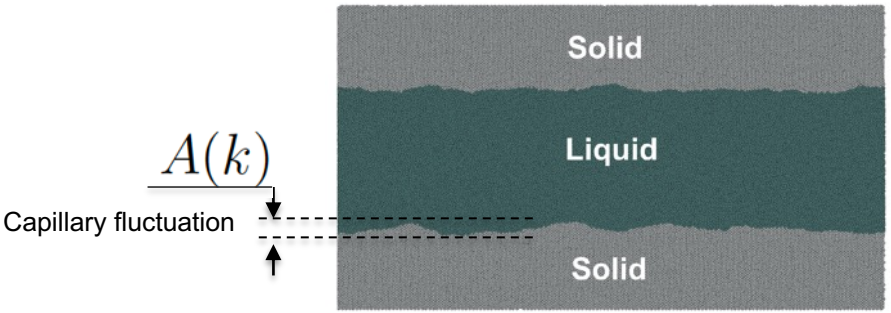
Capillary fluctuation method: $\langle |A(k)|^2 \rangle = \frac{k_B T}{lw\,(\gamma + \gamma'')\,k^2}$

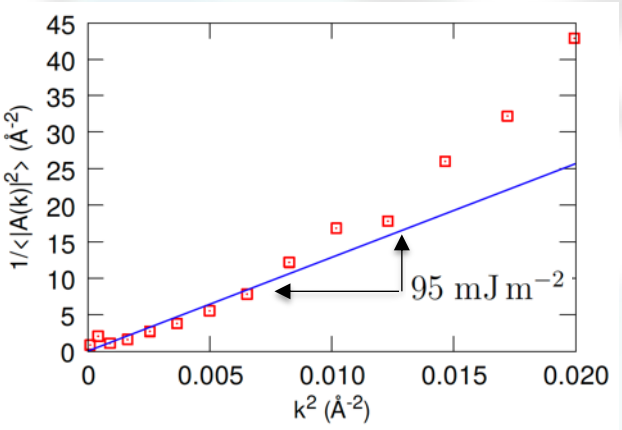
Surface tension, γ





Liquid-solid interface energy





Prediction of difficult to estimate interface energies is essential for AM applications

Example for Aluminum: Melt Properties

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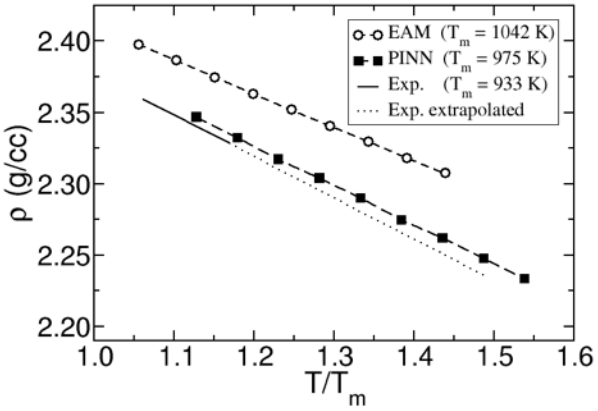
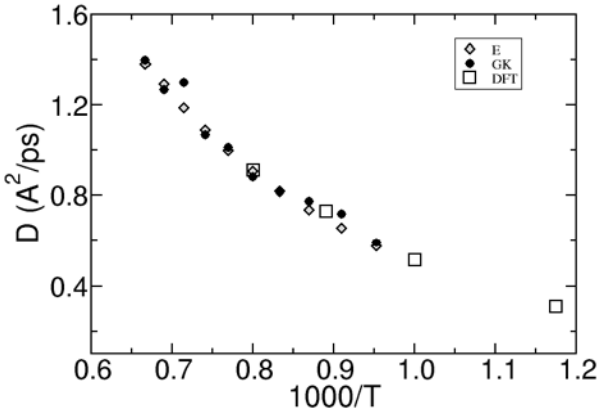
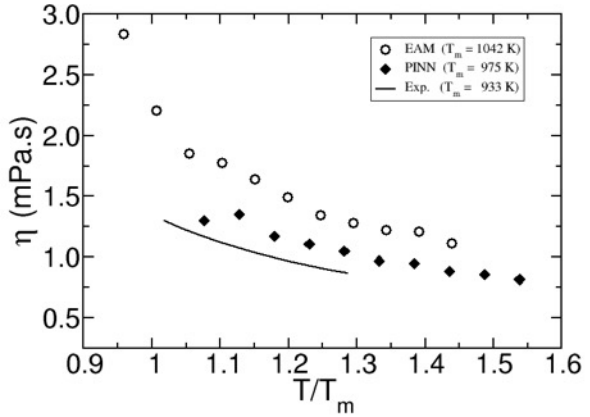
Density



Diffusion



Viscosity



EAM – Embedded Atom Method (Empirical) potential
PINN – Physically Informed Neural Network potential

Einstein: $D = \lim_{t\to\infty} \frac{1}{2t}\frac{1}{3N}\left\langle \sum_{i=1}^{N} [\vec{r}_i(t) - \vec{r}_i(0)]^2 \right\rangle$

$$\eta_{xy} = \frac{1}{Vk_BT}\int_0^\infty \langle P_{xy}(t)P_{xy}(0)\rangle dt\,; \quad P_{xy}(t) = \frac{d\Psi_{xy,i}(t)}{dt}$$

Green-Kubo: $D = \frac{1}{3N}\int_0^\infty \left\langle \sum_{i=1}^{N} \vec{v}_i(t) * \vec{v}_i(0) \right\rangle dt$

DFT: N. Jakse & A. Pasturel, Scientific Reports 3 (2013) 3135.

Accurate prediction of density, diffusivity, and viscosity is essential for AM applications

Computational Implementation of PINN

Exploring the recent advancements in supercomputer architectures

- PINN calculations are computationally highly demanding: ~ 3,000,000 floating point operations per atom
- High Performance Computing (HPC) implementation is strongly required
- ParaGrandMC code developed at NASA and NIA provides massively parallel computational platform for PINN (https://software.nasa.gov/software/LAR-19893-1)

NASA/LaRC midrange supercomputing K-cluster

Midrange supercomputing K-cluster provides learning environment for HPC development

Computational Implementation of PINN

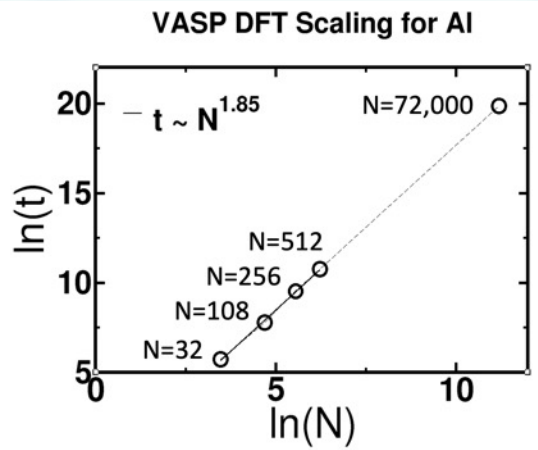
Test example on an aluminum crystal for 100 molecular dynamics (MD) time steps

Direct 1:1 comparison to DFT

N=500 100 MDS	EAM 16 cores	PINN 16 cores	DFT 32 nodes
Time, t	0.39 s	35 s	46,688 s
t/t_{EAM}	1	89	119,107

Larger scale beyond DFT capabilities

N=72,000 100 MDS	EAM	PINN	DFT 32 nodes extrapolated
16 cores	3.5 s (1)	528 s (151)	13.5 years
16 cores + V100	-	115 s (33)	-



PINN is slower than empirical potentials, but much faster than DFT without loss of accuracy

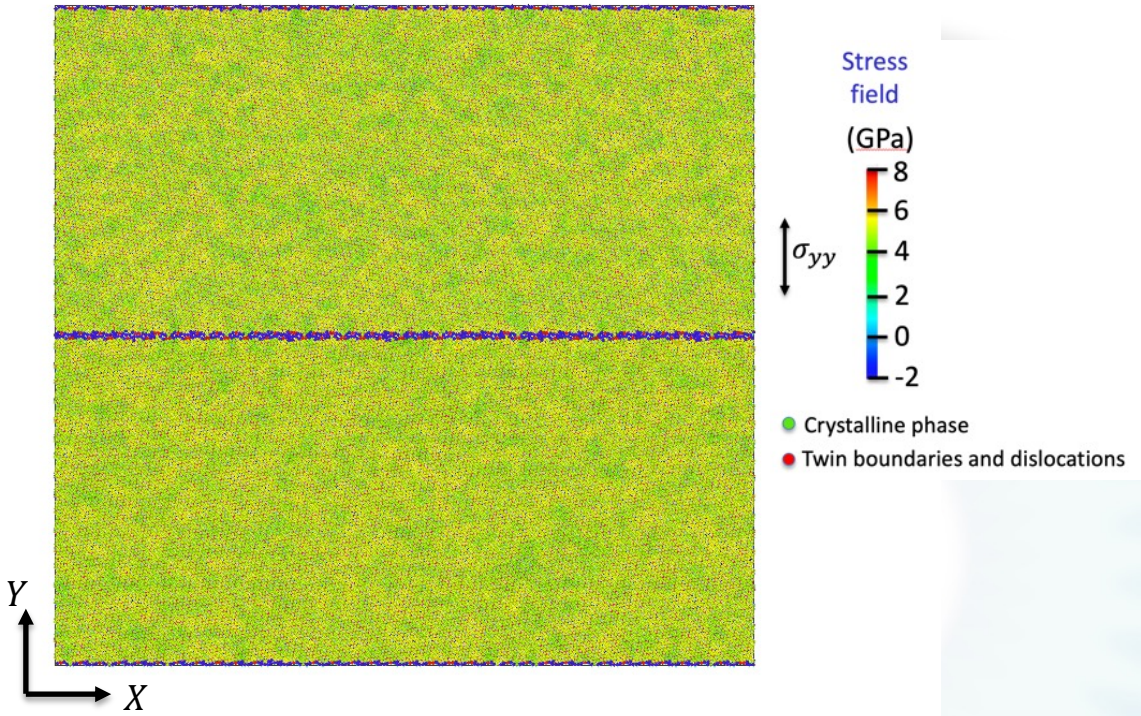
Computational Implementation of PINN

Simulation of a central crack nucleation along a grain boundary in aluminum using PINN potential

Crack growth simulation with DFT precision

433,000 atoms; 24 ps MD simulation
(12,000 MD time steps)
4 MPI nodes using (10 Skylake 6148 CPUs + V100 GPU) / node
14 cpu hours

ParaGrandMC code developed at NASA and NIA
(https://software.nasa.gov/software/LAR-19893-1)



High performance computing technologies allow for large scale PINN simulations

Conclusion

- Atomistic simulations provide fundamental understanding of materials behavior and help design new advanced materials
- Machine learning in atomistic simulations reproduces atomic forces with quantum mechanics precision at orders of magnitude lower computational cost
- Applied in additive manufacturing NN-based interatomic potential can accurately predict solid phase and melt properties of metallic alloys to guide process optimization
- Other PINN potentials under development for:
  - Additive Manufacturing: Ti, Ti-Al, Ti-Al-V (Ti-6Al-4V aerospace alloy) – NASA/LaRC
  - Semiconductor industry: Si, Si-C – GMU, NIST
  - Other: Ta, Cu-Ta – in collaboration with GMU

Acknowledgements

- NASA Transformational Tools and Technologies (T3) Project
- High-End Computing Capability Project – NASA Advanced Supercomputing Division: Gabriele Jost and Daniel Kokron
- NASA/LaRC midrange supercomputing K-cluster
- Cooperative agreement NNL09AA00A with the National Institute of Aerospace