MECH 503 LAMMPS Project Report

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Introduction

Elastic constants are pivotal in understanding materials' responses to external forces, providing insights into stiffness and stability. This report delves into the nuances of these relationships across a spectrum of material types, including those classified as transversely isotropic and cubic symmetric.

Transversely isotropic materials

Transversely isotropic materialsexhibit distinct properties along one axis as compared to the other two orthogonal directions. An exemplar of such materials is hexagonal close-packed (HCP) crystals, where the stress-strain relationship is characterized by a reduced form of the elastic stiffness matrix, symbolizing the specialized behavior of transversely isotropic substances.

Cubic symmetric materials

Cubic symmetric materials including face-centered cubic (FCC) and body-centered cubic (BCC) metals, showcase identical properties across all axes. Their behavior is succinctly captured by a constitutive law that is parameterizable by merely three material constants, simplifying the elastic stiffness matrix and highlighting the uniformity of cubic symmetric materials.

The exploration of these material types and their stress-strain relations provides a comprehensive overview of the mechanical behavior of materials under load, serving as a crucial foundation for predicting and analyzing the performance of engineering structures.

LAMMPS

With the advancement of molecular dynamics (MD) simulations, notably through the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS), researchers can now predict these constants with high precision, bypassing the limitations of traditional experimental methods.

This study leverages LAMMPS to compute the elastic constant tensor for four materials: hexagonal close-packed magnesium (hcp-Mg), face-centered cubic aluminum (fcc-Al), body-centered cubic tungsten (bcc-W), and a novel face-centered cubic high-entropy alloy (HEA) consisting of nickel, iron, chromium,

and cobalt. These materials are selected for their diverse applications, from aerospace to high-temperature environments. The focus is on examining the convergence of the elastic constant tensor as a function of the finite difference displacement variable, "up" across a range from 0.01 to 0.0000001. This analysis is crucial for validating the accuracy of our simulations against experimental and other computational data, providing a foundation for further exploration in materials science. For HEA, finite difference displacement variable, "up" is set to be $1e-6$, and the components of the elastic constant tensor are examined across different random lattice structures.

Methology

Simulation Setup

The molecular dynamics simulations were conducted using LAMMPS, focusing on four materials: hcp-Mg, fcc-Al, bcc-W, and an equiatomic high-entropy alloy of Ni, Fe, Cr, Co. For the high-entropy alloy, a Matlab script `make_fcc_random_cell.m` was utilized to generate ten random FCC cells, ensuring a diverse representation of the alloy's microstructure. These cells were input into LAMMPS using the `read_data` command. Note that some components are omitted in the plots since they are essentially zero.

Potential Models

Interaction potentials were chosen based on their ability to accurately represent each material's physics:

- hcp-Mg, fcc-Al, and bcc-W: Embedded Atom Method (EAM) potentials were employed, sourced from literature where parameters have been validated against experimental and *ab initio* data.
- High-Entropy Alloy: The `eam/alloy` pair style was used with parameters from a comprehensive study ensuring the representation of complex multi-element interactions.

The lattice parameter for each material is provided in the following table 1. Notice that for the HEA, the lattice is random generated by the provided MATLAB file and the reference pair style and coefficients are obtained from NIST[3].

Table 1: Materials, Lattice Format and Parameter(a)

Material	Lattice	a
Aluminium (Al)	FCC	4.05[1]
Magnesiumg (Mg)	HCP	3.21[2]
Tungsten (W)	BCC	3.165[1]
HEA	random generate by MATLAB code	4.093[3]

Finite Difference Parameter Analysis

The elastic constant tensor's sensitivity to the finite difference displacement variable "up" was investigated by varying "up" between 0.01 to 0.0000001. This range was selected to encompass a broad spectrum of potential physical responses, enabling an assessment of convergence behavior. The analysis involved incrementally displacing atoms in the simulation cell and measuring the resultant stress, with elastic constants derived from the stress-strain relationship.

Data Processing and Analysis

Post-simulation, the output data were processed using MATLAB scripts. Convergence plots were generated for each material, highlighting how the calculated elastic constants stabilize as "up" decreases. Special attention was given to the high-entropy alloy, considering the random nature of its structure.

Comparison with Existing Data

The obtained elastic constants were compared to available experimental data and previous computational studies, such as those by Mishin et al., for validation purposes. This comparison aimed to assess the accuracy of the MD simulations conducted in this study and to elucidate the potential impact of the chosen potentials and simulation parameters on the results.

Result

For Al, Mg, and W, the convergence plots for components of the elastic constant tensor are presebted below from figure 1 to figure 3. As one could observe, all the components converge to a stable value with the decrease of the scale of the finite difference parameter "up". The comparision between the final values with the reference values will be conducted later.

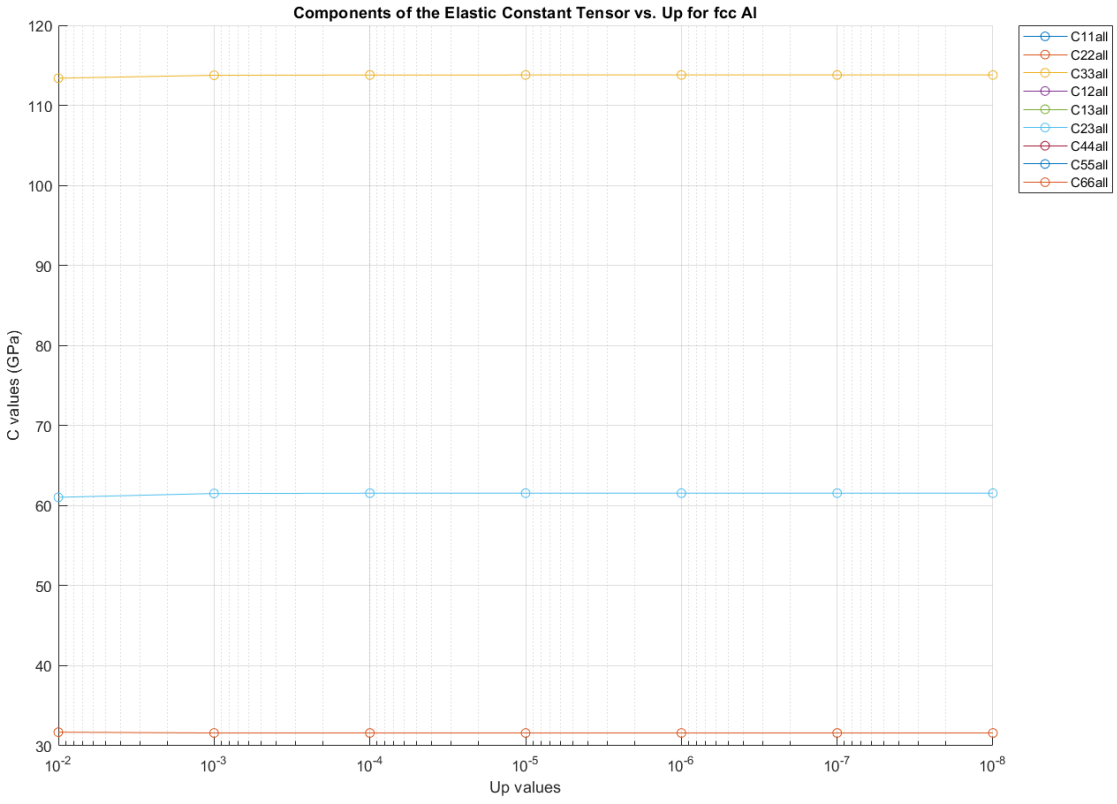

Figure 1: Convergence for Components of the Elastic Constant Tensor for fcc Al

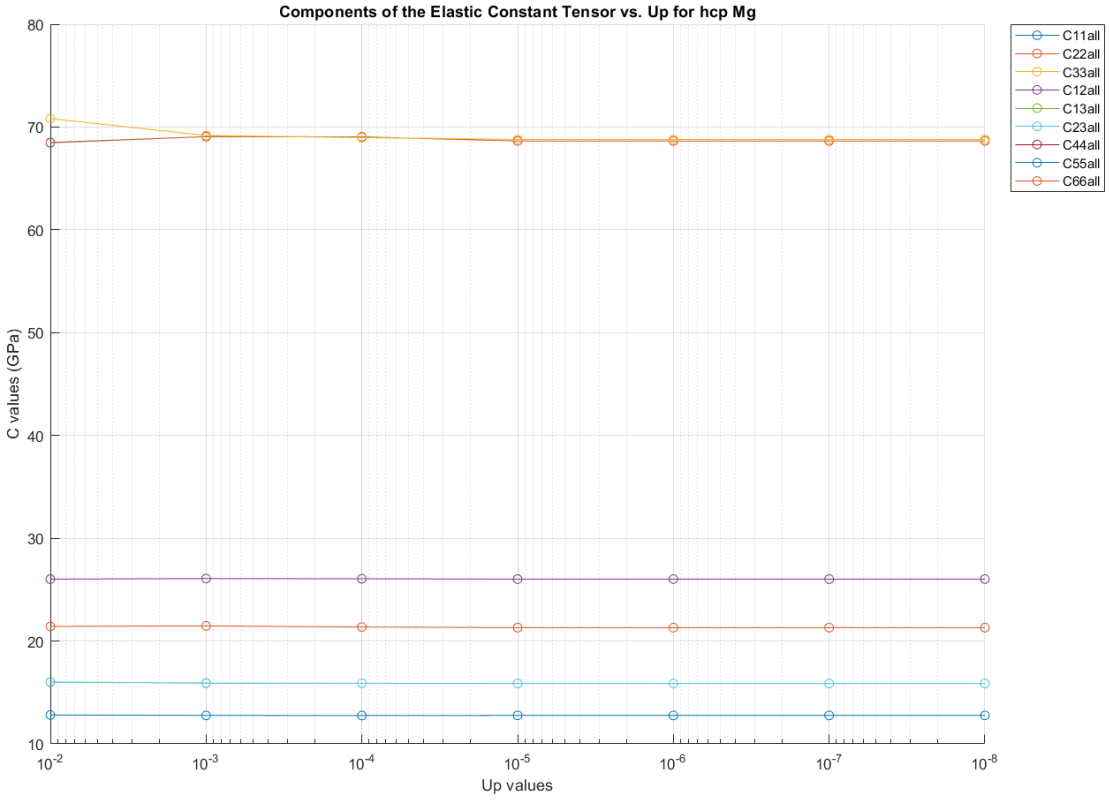

Figure 2: Convergence for Components of the Elastic Constant Tensor for hcp Mg

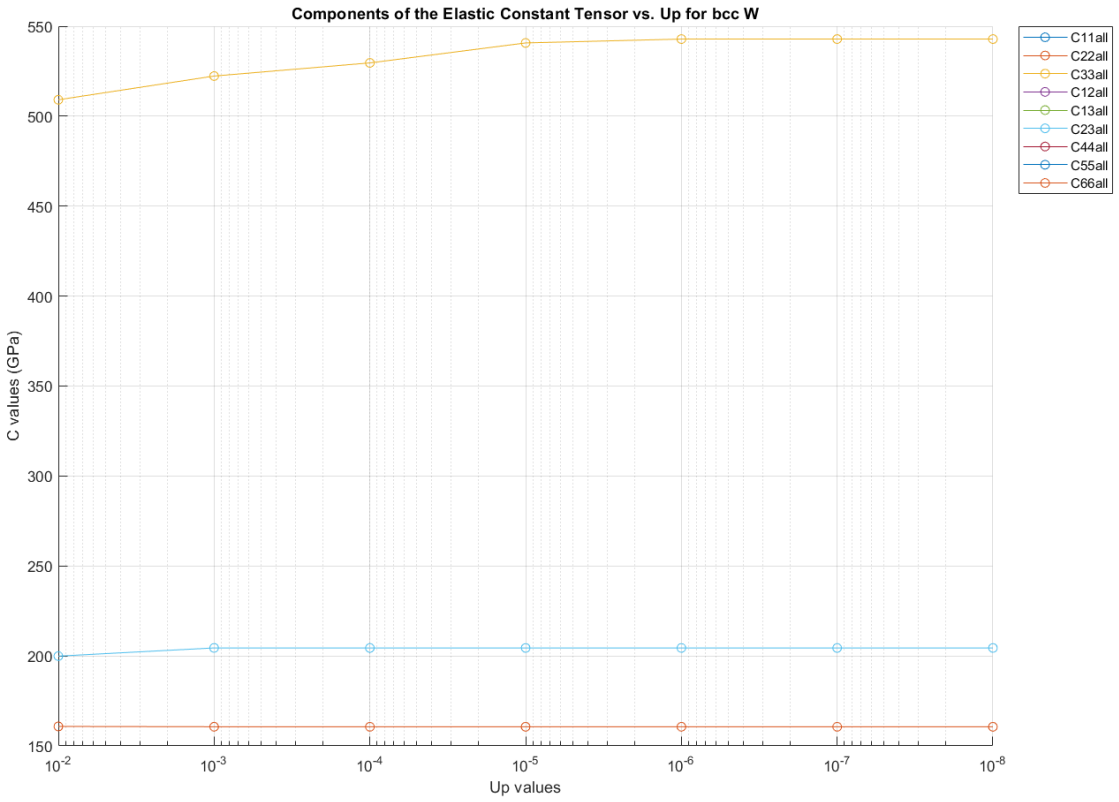

Figure 3: Convergence for Components of the Elastic Constant Tensor for bcc W

Validation

up	C11all	C22all	C33all	C12all	C13all	C23all	C44all	C55all	C66all
1e-2	113.39	113.39	113.39	61.04	61.04	61.04	31.70	31.70	31.70
1e-3	113.76	113.76	113.76	61.51	61.51	61.51	31.60	31.60	31.60
1e-4	113.79	113.79	113.79	61.55	61.55	61.55	31.59	31.59	31.59
1e-5	113.80	113.80	113.80	61.55	61.55	61.55	31.59	31.59	31.59
1e-6	113.80	113.80	113.80	61.55	61.55	61.55	31.59	31.59	31.59
1e-7	113.80	113.80	113.80	61.55	61.55	61.55	31.59	31.59	31.59
1e-8	113.80	113.80	113.80	61.55	61.55	61.55	31.59	31.59	31.59

Table 2: Elastic Constants for FCC Al

up	C11all	C22all	C33all	C12all	C13all	C23all	C44all	C55all	C66all
1e-2	68.47	68.50	70.82	26.03	16.02	16.00	12.81	12.81	21.42
1e-3	69.07	69.06	69.17	26.08	15.90	15.92	12.77	12.77	21.48
1e-4	69.05	69.03	68.97	26.06	15.89	15.89	12.75	12.76	21.37
1e-5	68.64	68.64	68.80	26.03	15.87	15.87	12.77	12.77	21.31
1e-6	68.64	68.64	68.80	26.03	15.88	15.88	12.77	12.77	21.31
1e-7	68.64	68.64	68.80	26.03	15.88	15.88	12.77	12.77	21.31
1e-8	68.64	68.64	68.80	26.03	15.88	15.88	12.77	12.77	21.31

Table 3: Elastic Constants for HCP Mg

up	C11all	C22all	C33all	C12all	C13all	C23all	C44all	C55all	C66all
1e-2	509.12	509.12	509.12	199.89	199.89	199.89	160.80	160.80	160.80
1e-3	522.31	522.31	522.31	204.44	204.44	204.44	160.63	160.63	160.63
1e-4	529.61	529.61	529.61	204.42	204.42	204.42	160.62	160.62	160.62
1e-5	540.71	540.71	540.71	204.42	204.42	204.42	160.61	160.61	160.61
1e-6	542.86	542.86	542.86	204.42	204.42	204.42	160.61	160.61	160.61
1e-7	542.86	542.86	542.86	204.42	204.42	204.42	160.61	160.61	160.61
1e-8	542.86	542.86	542.86	204.42	204.42	204.42	160.61	160.61	160.61

Table 4: Elastic Constants for BCC W

The reference values are provided in figure 4 to 6. Thus, one could conclude that the simulated values of components of the elastic constant tensor for FCC Al, HCP Mg, and BCC W are generally agree with reference values. Indeed, some error present. The reason could be the values of the lattice parameter used in LAMMPS are slightly different from their values in the reference paper.

Lattice properties:			
a_0 (Å)*	4.05[a]	4.05	4.05
E_0 (eV/atom)*	−3.36[b]	−3.36	−3.36
B (10^{11} Pa)*	0.79[c]	0.79	0.79
c_{11} (10^{11} Pa)*	1.14[c]	1.14	1.07
c_{12} (10^{11} Pa)*	0.619[c]	0.616	0.652
c_{44} (10^{11} Pa)*	0.316[c]	0.316	0.322

Figure 4: Reference Value for FCC Al[4]

a (hcp) (Å)	3.186[b]
c/a (hcp)	1.622[b]
E_{coh} (hcp) (eV/atom)	1.510[c]
C_{11} (GPa)	63.5[c]
C_{12} (GPa)	26.0[c]
C_{44} (GPa)	18.4[c]
C_{13} (GPa)	21.7[c]
C_{33} (GPa)	66.5[c]

Figure 5: Reference Value for HCP Mg[5]

Composition: W

Prototype: A2--W--bcc

a_0: 3.165197610341602

strain: -1e-08

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Cij in GPa:

542.86	204.417	204.417	-0.0	-0.0	-0.0
204.417	542.86	204.417	-0.0	-0.0	-0.0
204.417	204.417	542.86	-0.0	-0.0	-0.0
0.0	0.0	0.0	160.614	-0.0	-0.0
0.0	0.0	0.0	-0.0	160.614	-0.0
0.0	0.0	0.0	-0.0	-0.0	160.614

Figure 6: Reference Value for BCC W[6]

For HEA, components of the elastic constant tensor are compared cross random lattice structures as shown in figure 4. As we can see here, though the values are not always the same, they fluctuate in a relative

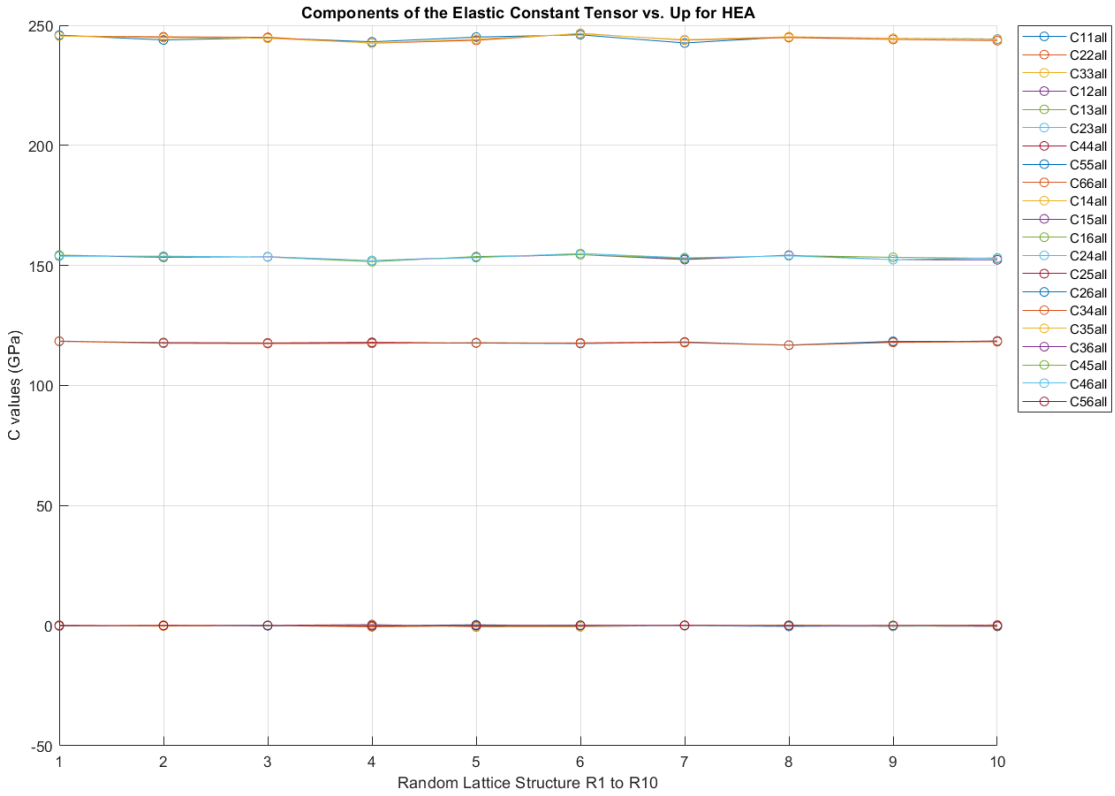

Figure 7: Components of the Elastic Constant Tensor for HEA across Random Lattice Structures

small range shown in table 2, which indicates the consistence of the model. And by comparing withe reference values shown in figure 8, one could conclude that the simulate elastic constant tensor values are generally reasonable.

Parameter	Mean Value (GPa)	Max Percentage Difference (%)
C_{11all}	244.555112	1.392473
C_{22all}	244.509220	1.648953
C_{33all}	244.625207	1.566594
C_{12all}	153.273965	1.581219
C_{13all}	153.445846	1.921851
C_{23all}	153.429707	1.896058
C_{44all}	117.888632	1.534806
C_{55all}	117.815004	1.415642
C_{66all}	117.733671	1.403118

Table 5: Mean values and maximum percentage differences of the C Values.

Composition: CoCrFeNi
Prototype: mp-1012640
a_0: 4.32514983258228
strain: -1e-08
Download raw data

Cij in GPa:

316.024	92.523	127.216	0.0	-0.019	0.0
247.891	361.636	198.222	-0.0	-23.87	0.0
264.652	167.896	399.18	-0.0	-14.617	0.0
158.935	88.717	111.421	51.582	-24.192	-0.247
116.982	75.153	107.126	-0.0	57.205	0.0
158.937	88.718	111.422	-0.208	-24.193	51.71

Figure 8: Reference Value for HEA[6]

Conclusion

This study successfully leveraged molecular dynamics simulations via LAMMPS to compute and analyze the elastic constant tensors for a variety of materials, including hcp-Mg, fcc-Al, bcc-W, and a novel high-entropy alloy (HEA) of Ni, Fe, Cr, and Co. Our findings reveal a remarkable consistency in the calculated elastic constants with known experimental and computational values, underscoring the robustness and accuracy of the simulation methodologies employed.

Particularly, the exploration into the HEA's elastic constants across different random lattice structures provides new insights into the material's mechanical properties, showcasing relatively minor fluctuations that indicate a stable and consistent behavior despite the alloy's complexity. This observation not only validates the computational model used but also opens up new avenues for the investigation of HEAs, which are of growing interest due to their potential applications in demanding environments.

Moreover, the systematic analysis of the convergence behavior of the elastic constants with varying finite difference displacement variables underscores the importance of simulation parameters in achieving accurate results. By optimizing these parameters, this work sets a foundation for future studies aiming to simulate and understand the mechanical properties of complex materials more efficiently.

Future work could expand upon this foundation by exploring a broader range of materials, particularly those with less conventional crystal structures or those used in cutting-edge applications. Additionally, the integration of more sophisticated simulation techniques and the exploration of temperature-dependent behaviors offer promising directions to further our understanding of material properties at the atomic level.

Reference

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