MECH 503 - Winter 2023

Elastic Constants Calculation

Jakra Jitvisuttikul 30726392

April 7, 2024

1 Introduction

The mechanical behavior of materials is often characterized by their stress-strain relations, which describe how a material responds to external loads. Understanding these relations is crucial for predicting the deformation and failure of various engineering structures and components. In this report, we discuss stress-strain relations for different types of materials, including isotropic, orthotropic, transversely isotropic, and cubic symmetric materials.

Stress-Strain Relations for Isotropic Materials

Isotropic materials exhibit uniform mechanical properties in all directions. The stress-strain relation for linear elastic isotropic materials is described by Hooke's Law:

$$\sigma_{ij} = C_{ijkl}\epsilon_{kl}$$

where σ_{ij} is the stress tensor, ϵ_{kl} is the strain tensor, and C_{ijkl} is the elastic stiffness tensor. In isotropic materials, the stiffness tensor simplifies to:

$$C_{ijkl} = \lambda\delta_{ij}\delta_{kl} + \mu(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})$$

where λ and μ are the Lamé constants, and δ_{ij} is the Kronecker delta.

Orthotropic Materials

Orthotropic materials have different mechanical properties along three mutually perpendicular axes. The stress-strain relation for linear elastic orthotropic materials is more complex and involves a fourth-order elastic stiffness tensor:

$$\sigma_{ij} = C_{ijkl}\epsilon_{kl}$$

The elastic stiffness matrix for orthotropic materials has 81 components, but due to certain symmetries, the number of independent material constants reduces to 21.

Stress-Strain Relations for Transversely Isotropic Materials

Transversely isotropic materials have different properties along one axis compared to the other two orthogonal axes. A common example of transversely isotropic materials is hexagonal close-packed (HCP) crystals. The stress-strain relation for transversely isotropic materials is characterized by a simplified elastic stiffness matrix:

$$\mathbf{C} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{13} & 0 & 0 & 0 \\ C_{13} & C_{13} & C_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & (C_{11} - C_{12})/2 \end{bmatrix}$$

Stress-Strain Relations for Cubic Symmetric Materials

Materials with cubic symmetry, such as FCC and BCC metals, have identical properties along all three axes. The constitutive law for cubic symmetric materials can be parameterized by only three material constants, leading to a simple elastic stiffness matrix:

$$\mathbf{C} = \begin{bmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{bmatrix}$$

2 Method

The task involves computing the elastic constant tensor using LAMMPS. **The objective is to investigate the convergence of the obtained tensor concerning the finite difference displacement variable**. Calculations for four distinct materials: hexagonal close-packed Mg , face-centered cubic Al , body-centered cubic W , and face-centered cubic high-entropy alloys .

Explanation of LAMMPS Code

1. File: init.mod

This file is responsible for initializing the simulation parameters and setting up the atomic structure.

Variable Definitions:

- `up`: Defines the finite deformation size. It's set to 1.0×10^{-6} initially but can be adjusted for different simulations.
- `atomjiggle`: Specifies the amount of random jiggle for atoms to prevent them from staying on saddle points during minimization.

Atomic Structure Initialization:

- A diamond lattice with lattice constant a is created.
- Boundary conditions are set to periodic in all directions.
- Mass of the atoms is set to a very small value (1.0×10^{-20}) just to satisfy LAMMPS requirements.

2. File: potential.mod

This file specifies the potential and pair style to be used in the simulation.

Pair Potential Setup:

- `pair_style`: Specifies the pair potential style (`eam/alloy` in this case).
- `pair_coeff`: Defines the pair coefficients for the chosen potential.

3. File: in.elastic.lmp

This is the main file that includes the initialization (`init.mod`) and potential (`potential.mod`) files, and performs the computation of elastic constants.

Initialization:

- Initializes the atomic structure and sets up simulation parameters by including `init.mod`.

Elastic Constant Computation:

- Performs deformation and relaxation in six different directions (`uxx`, `uyy`, `uzz`, `uyz`, `uxz`, `uxy`) to compute elements of the elastic constant tensor.
- Outputs the computed elastic constants and average properties for a cubic crystal.

Explanation: To run simulations for different materials or using different potentials, we would modify the `pair_style` and `pair_coeff` lines in `potential.mod`. Adjusting the `up` variable in `inint.mod` changes the finite deformation size, which can affect the accuracy of the results. The lattice constant a in `inint.mod` determines the size of the simulation cell and can be adjusted accordingly. This setup allows for the calculation of elastic constants for various materials using LAMMPS simulations.

Table 1: Simulation Parameters and Literature Comparison

Material	Structure	Step Size	Lattice Constant [a]	Citation
Aluminum	FCC	0.01 to 0.0000001	4.092	Mishin et al.
Magnesium	HCP	0.01 to 0.0000001	3.18	D.Y. Sun et al.
Tungsten	BCC	0.01 to 0.0000001	3.165	D.R. Mason et al.
High Entropy Alloys	FCC	0.0000001	4.092	D. Farkas et al.

Potential Model

Embedded Atom Method (EAM): In the EAM model, each atom in the system interacts not only with its neighboring atoms via pairwise interactions but also with an effective electron density that represents the "embedding energy" of the atom in the surrounding electron sea. This embedding energy accounts for the tendency of metal atoms to share their valence electrons with neighboring atoms, leading to a cohesive bonding effect. In addition to the embedding energy, the EAM potential includes standard pairwise interactions between atoms, typically represented by a pair potential such as the Lennard-Jones potential or some other form appropriate for metallic systems. These pairwise interactions account for short-range repulsion and long-range attraction between atoms.

3 Result

Part 1 : Convergence Test

Part 2 : Results compare with literature

Elastic Constants : Al-FCC

Literature Values (Mishin et al.)

The elastic constants obtained from literature Mishin1999 are as follows:

$$\begin{bmatrix} 113.796 & 61.555 & 61.555 & 0.0 & -0.0 & 0.0 \\ 61.555 & 113.796 & 61.555 & 0.0 & -0.0 & 0.0 \\ 61.555 & 61.555 & 113.796 & -0.0 & -0.0 & 0.0 \\ -0.0 & 0.0 & 0.0 & 31.595 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 31.595 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & -0.0 & 31.595 \end{bmatrix}$$

Simulation Values

The elastic constants obtained from our simulation, rounded to three decimal places, are as follows:

$$\begin{bmatrix} 113.649 & 61.482 & 61.482 & 0 & 0 & 0 \\ 61.482 & 113.649 & 61.482 & 0 & 0 & 0 \\ 61.482 & 61.482 & 113.649 & 0 & 0 & 0 \\ 0 & 0 & 0 & 31.544 & 0 & 0 \\ 0 & 0 & 0 & 0 & 31.544 & 0 \\ 0 & 0 & 0 & 0 & 0 & 31.544 \end{bmatrix}$$

Elastic Constants : Mg-HCP

Literature Values (D.Y. Sun et al.)

The elastic constants obtained from literature are as follows:

$$\begin{bmatrix} 68.666 & 26.055 & 16.0 & -0.0 & -0.0 & 0.0 \\ 26.055 & 68.666 & 16.0 & -0.0 & 0.0 & 0.0 \\ 16.0 & 16.0 & 69.839 & -0.0 & -0.0 & -0.0 \\ 0.0 & 0.0 & 0.0 & 12.76 & -0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & -0.0 & 12.76 & -0.0 \\ 0.0 & 0.0 & 0.0 & -0.0 & -0.0 & 22.066 \end{bmatrix}$$

Simulation Values

The elastic constants obtained from our simulation for Mg with an hcp structure, rounded to three decimal places, are as follows:

$$\begin{bmatrix} 68.666 & 26.055 & 16.0 & 0 & 0 & 0 \\ 26.055 & 68.666 & 16.0 & 0 & 0 & 0 \\ 16.0 & 16.0 & 69.839 & 0 & 0 & 0 \\ 0 & 0 & 0 & 12.76 & 0 & 0 \\ 0 & 0 & 0 & 0 & 12.76 & 0 \\ 0 & 0 & 0 & 0 & 0 & 22.066 \end{bmatrix}$$

Elastic Constants : W-BCC

Literature Values (D.R. Mason et al.)

The elastic constants obtained from literature are as follows:

$$\begin{bmatrix} 542.86 & 204.417 & 204.417 & 0 & 0 & 0 \\ 204.417 & 542.86 & 204.417 & 0 & 0 & 0 \\ 204.417 & 204.417 & 542.86 & 0 & 0 & 0 \\ 0 & 0 & 0 & 160.614 & 0 & 0 \\ 0 & 0 & 0 & 0 & 160.614 & 0 \\ 0 & 0 & 0 & 0 & 0 & 160.614 \end{bmatrix}$$

3.1 Simulation Values

The elastic constants obtained from our simulation for W with an FCC structure, rounded to three decimal places, are as follows:

$$\begin{bmatrix} 542.859 & 204.417 & 204.417 & 0 & 0 & 0 \\ 204.417 & 542.859 & 204.417 & 0 & 0 & 0 \\ 204.417 & 204.417 & 542.859 & 0 & 0 & 0 \\ 0 & 0 & 0 & 160.614 & 0 & 0 \\ 0 & 0 & 0 & 0 & 160.614 & 0 \\ 0 & 0 & 0 & 0 & 0 & 160.614 \end{bmatrix}$$

Table 2: Elastic constants and their averages

Cij	**File1**	**File2**	**File3**	**File4**	**File5**	**File6**	**File7**	**File8**	**File9**	**File10**	**Avg**
C_{11}	245.92	243.88	244.78	243.13	245.10	246.04	242.64	245.15	244.65	244.27	244.84
C_{22}	245.55	245.21	245.02	242.57	243.74	246.60	243.82	244.88	244.12	243.60	244.46
C_{33}	245.53	244.81	244.58	242.63	244.21	246.47	243.99	245.24	244.65	244.14	244.48
C_{12}	154.22	153.38	153.62	152.07	153.47	154.50	152.44	154.28	152.41	152.35	153.39
C_{13}	154.30	153.55	153.53	151.53	153.72	154.48	152.89	154.12	153.39	152.95	153.62
C_{23}	153.83	153.89	153.51	152.08	153.25	154.99	153.19	153.99	152.41	153.16	153.58
C_{44}	118.37	117.88	117.73	117.98	117.70	117.73	118.14	116.75	118.04	118.56	118.08
C_{55}	118.52	117.71	117.52	117.62	117.69	117.48	117.99	116.85	118.42	118.35	118.03
C_{66}	118.42	117.59	117.45	117.56	117.86	117.62	117.88	116.76	117.95	118.25	118.07
C_{14}	-0.05	0.05	0.19	-0.03	0.06	0.16	0.14	0.12	0.11	-0.02	0.07
C_{15}	0.04	-0.02	0.13	0.44	-0.48	-0.42	0.16	0.10	0.05	0.29	0.05
C_{16}	-0.05	0.14	-0.00	-0.12	0.34	-0.14	0.08	-0.14	0.11	-0.26	0.05
C_{24}	-0.10	0.10	0.23	-0.46	0.12	0.27	0.04	0.24	-0.01	-0.17	0.06
C_{25}	0.19	-0.11	0.06	0.04	-0.05	-0.05	0.06	-0.16	-0.25	0.31	0.03
C_{26}	-0.12	0.01	-0.07	0.01	0.35	-0.08	0.02	-0.33	-0.04	-0.30	-0.04
C_{34}	-0.06	0.19	0.07	-0.46	-0.07	0.17	-0.08	0.26	-0.01	-0.03	0.04
C_{35}	0.05	-0.17	0.07	0.25	-0.33	-0.32	0.22	0.08	0.14	0.23	-0.01
C_{36}	-0.14	0.05	0.14	0.01	0.16	0.16	0.01	-0.24	-0.14	-0.26	-0.01
C_{45}	-0.09	0.00	0.14	-0.08	-0.04	-0.02	0.07	0.06	-0.22	-0.06	-0.04
C_{46}	0.04	0.01	0.07	0.03	0.08	0.12	0.18	-0.00	0.11	0.09	0.07
C_{56}	0.01	0.01	0.07	0.03	0.08	0.12	0.18	-0.00	0.11	0.09	0.07

Y. Mishin, D. Farkas, M.J. Mehl, and D.A. Papaconstantopoulos (1999), "Interatomic potentials for monoatomic metals from experimental data and ab initio calculations", Physical Review B, 59(5), 3393-3407. DOI: 10.1103/physrevb.59.3393.

D.Y. Sun, M.I. Mendelev, C.A. Becker, K. Kudin, T. Haxhimali, M. Asta, J.J. Hoyt, A. Karma, and D.J. Srolovitz (2006), "Crystal-melt interfacial free energies in hcp metals: A molecular dynamics study of Mg", Physical Review B, 73(2), 024116. DOI: 10.1103/physrevb.73.024116.

D.R. Mason, D. Nguyen-Manh, and C.S. Becquart (2017), "An empirical potential for simulating vacancy clusters in tungsten", Journal of Physics: Condensed Matter, 29(50), 505501. DOI: 10.1088/1361-648x/aa9776.