ETH Zurich
Department of Mechanical and Process Engineering
Statistical Mechanics of Elasticity
Exercise 7 - Summer 2007

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Center of Mechanics
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Useful Definitions

Simple lattice

A *simple lattice* or *Bravais lattice* is an infinite set of points in d-dimensional space generated by the translation of a single point $\mathbf{o}$ through d linearly independent lattice vectors $\mathbf{a}_i$, i.e.

$$\mathcal{L}(\mathbf{a}_i, \mathbf{o}) = \{\mathbf{x} \,|\mathbf{x} = \mathbf{o} + \ell_i \mathbf{a}_i, \quad \ell_i \in \mathbb{Z}, \quad i = 1, .., d\}\,. \tag{1}$$

Multilattice

A *multilattice* or *n-lattice* is defined as the superposition of n Bravais lattices that have the same lattice vectors and that are shifted by $n-1$ shifts $\mathbf{p}$. For a $2-lattice$ one gets

$$\mathcal{L}(\mathbf{a}_i, \mathbf{o}, \mathbf{p}) = \mathcal{L}(\mathbf{a}_i, \mathbf{o}) \bigcup \mathcal{L}(\mathbf{a}_i, \mathbf{o} + \mathbf{p}). \tag{2}$$

Cauchy-Born Hypothesis for simple lattices

The Cauchy-Born hypothesis assumes that lattice vectors in a deformed crystalline solid behave like line elements and are deformed according to the deformation gradient, i.e.

$$\mathbf{a}_i = \mathbf{F}\mathbf{a}_i^o, \tag{3}$$

where $\mathbf{a}_i^o$ are the lattice vectors in the reference configuration.

Cauchy-Born Hypothesis for multilattices

As opposed to the simple lattice, deformations in a multilattice are not completely described by the deformation of the lattice vectors: The deformation of the shifts $\mathbf{p}_j$ also has to be specified. However, these shifts are not linked to the macroscopic deformation and constitute internal degrees of freedom of the lattice. They are hence determined from energy minimization, i.e.

$$\begin{aligned} \mathbf{a}_i \quad &= \quad \mathbf{F}\mathbf{a}_i^o \text{ (as for the simple lattice)}, \\ \mathbf{p} \quad &\textit{from} \quad \min_{\mathbf{p}} \Psi(\mathbf{a}_i, \mathbf{p}), \end{aligned} \tag{4}$$

where $\Psi(\mathbf{a}_i, \mathbf{p})$ is the Helmholtz free energy of the lattice that coincides with its potential energy at zero temperature.

Problem 1 - Fitting of Lennard-Jones parameters for Xenon

Consider Xenon at a very low temperature, $t \approx 0K$. From measurements you know that Xenon exhibits an *fcc* structure , that the lattice parameter is given by $L = 6.13$ Å and that the cohesevie energy of the lattice is given by $0.17eV/$atom. Assuming the interactions between Xenon atoms can be modelled using Lennard-Jones potentials of the form

$$u(r) = u_o \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right] \tag{5}$$

determine the parameters σ and u_o from the measured values. To do so analytically, consider only next-nearest neighbors when computing the potential energy.

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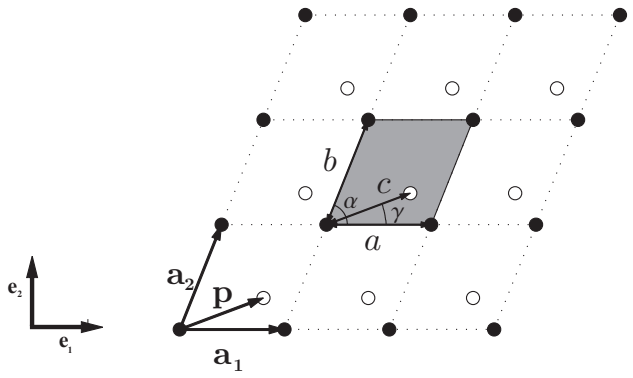

Figure 1: The parametrization of the 2D diatomic lattice.

Homework 1 - Deformation of lattice with internal shift

Consider a diatomic lattice consisting of two atomic species A and B. Interactions between atoms are governed by Lennard-Jones potentials of the form

$$u_{\alpha\beta}(r) = u^o_{\alpha\beta}\left[\left(\frac{\sigma_{\alpha\beta}}{r}\right)^{12} - \left(\frac{\sigma_{\alpha\beta}}{r}\right)^{6}\right] \tag{6}$$

where the interaction are given by $u^o_{AA} = u^o_{BB} = 1U_o$, $u^o_{AB} = 10U_o$ (this is unrealistic but amplifies the effect we are interested in) and $\sigma_{AA} = \sigma_{BB} = 1\sigma_o$, $\sigma_{AB} = 0.45\sigma_o$.

Goal of the exercise is to see how the minimization of the internal shift influences the potential energy of the lattice during uniform expansion. To do so, carry out the following steps, preferebly in MATLAB:

a) Parametrize the diatomic lattice (i.e. the lattice vectors $\mathbf{a}_i$ and the shift $\mathbf{p}$) as shown in Figure (1) using five parameters, i.e. compute

$$\mathbf{a}_i = \mathbf{a}_i(a, b, c, \alpha, \gamma) \text{ and } \mathbf{p} = \mathbf{p}(a, b, c, \alpha, \gamma). \tag{7}$$

b) Set up a function *pot.m* that calculates the potential energy of a unit cell (i.e. an A and a B atom) from given lattice vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ and the shift $\mathbf{p}$ taking into account all interactions of atoms that are in

$$\{\mathbf{x}\,|\mathbf{x} - \mathbf{x}_o = \ell_1\mathbf{a}_1 + \ell_2\mathbf{a}_2, \quad |\ell_1|, |\ell_2| \leq 6\}, \tag{8}$$

where $\mathbf{x}_o$ are the members of the unit cell under consideration.

c) Use *fminsearch* (in MATLAB) to find minimum energy configurations of the lattice. *fminsearch* therefor requires you to pass it a starting vector, i.e. an initial guess for $(a, b, c, \alpha, \gamma)$. Carry out minimizations for the following starting configurations:

A) $(a, b, c, \alpha, \gamma) = (1.0, 1.0, 0.5, 1.0, 0.5)$

B) $(a, b, c, \alpha, \gamma) = (1.0, 1.0, 1.0, 1.0, 0.5)$

C) $(a, b, c, \alpha, \gamma) = (1.0, 1.0, 0.5, 1.0, 1.0)$

D) $(a, b, c, \alpha, \gamma) = (1.0, 2.0, 0.5, 0.5, 0.0)$

where all angles are given in radians. Plot all resulting configurations using the file *plotLattice.m* that is available online. Do the different results correspond to different phases? Compare both plots and resulting energies. Now chose the first computed minimum configuration as the reference configuration, i.e. set $\mathbf{a}_i^o$ and $\mathbf{p}^o$ to the computed minimizers.

d) The material in the obtained reference configuration is now subjected to a uniform dilatation according to

$$F_{ij}(\lambda) = \begin{pmatrix} \lambda & 0 \\ 0 & \lambda \end{pmatrix}. \tag{9}$$

Calculate and plot the energy $U(\mathbf{F}(\lambda))$ of the deformed lattice for $0.95 < \lambda < 1.2$ using steps of $\Delta\lambda = 0.001$. To do so,

A) assume that *both* the $\mathbf{a}_i$ *and* $\mathbf{p}$ deform according to the Cauchy-Born hypothesis.

B) assume that *only* the $\mathbf{a}_i$ deform according to the Cauchy-Born hypothesis and determine $\mathbf{p}$ for each value of λ from a minimization of the energy with respect to $\mathbf{p}(c, \gamma)$, i.e. with respect to (c, γ).

Compute and plot both energies $U(\mathbf{F}(\lambda))$ over λ in the same figure. Also generate plots of the two $c(\lambda)$ that are obtained by the two methods as well as the $\gamma(\lambda)$. To see what effects cause the deviations from "global Cauchy-Born", plot the lattice configurations with minimized $\mathbf{p}$ for $\lambda = 0.95$ and $\lambda = 1.2$.

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