Stability analysis and modelling the phase transition in BCC lattice

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Abstract

The stability of body-centered cubic (BCC) lattice is studied in the presented work. The material is considered to consist of particles, interacting by means of Morse potential, having one dimensionless parameter, which determines the behaviour of the material. The stability criterions for BCC lattice were obtained both in terms of this parameter and in terms of the Gruneisen parameter, which is the known macroparameter. The process of destruction of unstable BCC lattice was simulated numerically. The raise of Gruneisen parameter, predicted analytically was verified. The result, that BCC lattice transforms to FCC lattice was obtained numerically.

1 Introduction

A number of metals (such as iron, tantalum, niobium) have body-centered cubic (BCC) lattice. It is a simple lattice (e. g. it is congruous to itself shifted via vector, connecting any of its two nods). Different criterions of stability for this lattice were obtained in [2]–[4]. But all of these criterions were not verified. The purpose of this paper is to obtain a verifiable criterion, verify it and to predict the behavior of a material with BCC lattice, when it loses its stability. The main goal of the investigation is to describe the BCC–FCC transition, taking place in iron.

2 Basic data

The material is considered to be consisting of particles, interacting by pair potential. Morse potential is chosen to describe the interaction between particles, as it was done in [2, 3, 4]. This potential is given by formula

$$\Pi(r) = D\left[e^{-2\alpha(r-a)} - 2e^{-\alpha(r-a)}\right]. \tag{1}$$

The force of interatomic interaction is

$$F(r) = -\Pi'(r) = -2\alpha D\left[e^{-2\alpha(r-a)} - e^{-\alpha(r-a)}\right], \tag{2}$$

where r is a distance between interacting particles, D is a deepness of the potential well, α is a parameter, determining the width of the potential well, a is an equilibrium distance between two interacting particles. This potential has one dimensionless parameter $\alpha a = \aleph$. The potential (1) can be rewritten in terms of this parameter:

$$\Pi(r) = D\left[e^{-2\aleph(\frac{r}{a}-1)} - e^{-\aleph(\frac{r}{a}-1)}\right]. \tag{3}$$

Plots of the force for different values of $\aleph$ are presented at figure 1.

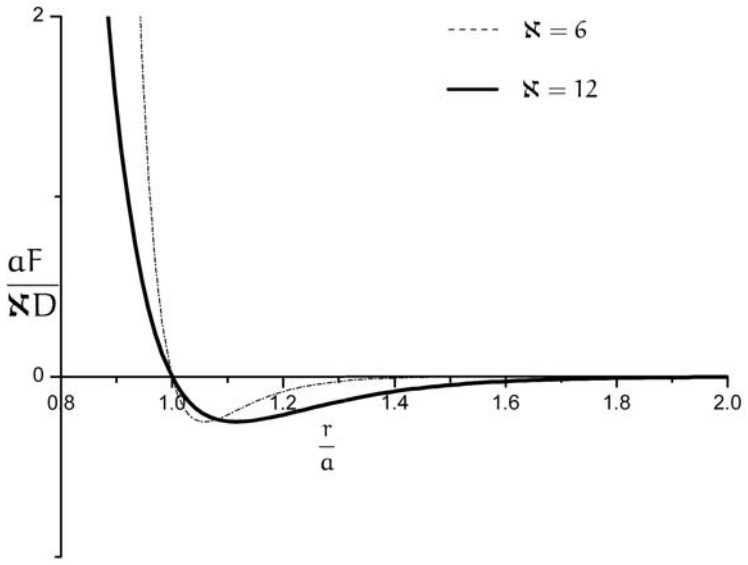

Figure 1: Graphs of force for different values of $\aleph$

The stability of the body-centered cubic (BCC) lattice is studied in the presented work. This lattice is a set of particles, located in the nods of a simple cubic lattice and in the center of symmetry of each cube. The stress tensor for this lattice, as for a simple one, can be written as following [1]:

$$\underline{\underline{\tau}} = \frac{1}{2V_0}\sum_{\beta}\frac{\Pi'(\underline{a}_\beta)}{a_\beta}\underline{a}_\beta\underline{a}_\beta, \tag{4}$$

where V_0 is a volume of an elementary cell (such a cell, containing one atom, that all the space can be filled out with it). The equilibrium condition can be written in the following form:

$$\underline{\underline{\tau}} = 0. \tag{5}$$

The stiffness tensor in the equilibrium position can be represented as in [1]

$${}^4\underline{\underline{C}} = \frac{1}{2V_0}\sum_{\beta}\left(\frac{\Pi''(a_\beta)}{a_\beta^2} - \frac{\Pi'(a_\beta)}{a_\beta^3}\right)\underline{a}_\beta\underline{a}_\beta\underline{a}_\beta\underline{a}_\beta. \tag{6}$$

The condition of the positive definiteness of the stiffness tensor was chosen as the stability condition.

3 Dependence of components of stiffness tensor on potential parameters. Stability criterion.

For the pair potential the stiffness tensor has only two independent components. Matrix, corresponding to this tensor in the basis $(\underline{e}_1, \underline{e}_2, \underline{e}_3)$ has the form

$$\underline{\underline{C}} \sim \begin{bmatrix} C_1 & C_2 & C_2 & 0 & 0 & 0 \\ C_2 & C_1 & C_2 & 0 & 0 & 0 \\ C_2 & C_2 & C_1 & 0 & 0 & 0 \\ 0 & 0 & 0 & C_2 & 0 & 0 \\ 0 & 0 & 0 & 0 & C_2 & 0 \\ 0 & 0 & 0 & 0 & 0 & C_2 \end{bmatrix}, \tag{7}$$

where

$$C_1 = \frac{1}{2V_0} \sum_\beta \left(\frac{\Pi''(a_\beta)}{a_\beta^2} - \frac{\Pi'(a_\beta)}{a_\beta^3} \right) \left(\underline{a}_\beta \cdot \underline{e}_1 \right)^4, \tag{8}$$

$$C_2 = \frac{1}{2V_0} \sum_\beta \left(\frac{\Pi''(a_\beta)}{a_\beta^2} - \frac{\Pi'(a_\beta)}{a_\beta^3} \right) \left(\underline{a}_\beta \underline{a}_\beta \cdot\cdot \underline{e}_1 \underline{e}_2 \right)^2 \tag{9}$$

From (7), it follows that the stability condition of positive definiteness of the stiffness tensor has the form:

$$C_1 > C_2 > 0 \tag{10}$$

The dependence of C_1 and C_2 on $\aleph$ is presented at figure 2. As one can see from this figure, there exists the critical value of $\aleph = \aleph_*$, such that for $\aleph < \aleph_*$ the BCC lattice is stable and for $\aleph > \aleph_*$ it is unstable. This critical value can be found numerically: $\aleph_* \cong 4.5176$. So, the criterion of stability in terms of parameter of potential (3) was obtained:

$$\aleph < \aleph* \cong 4.5176 \tag{11}$$

This criterion is convenient for numerical analysis but it can't be verified, because there exists a problem of determination of $\aleph$ for real materials. This leads to necessity in a criterion in terms of some macroscopic parameter.

4 Relation between $\aleph$ and the Gruneisen parameter. Reformulation of the stability criterion.

In [5] the expression of the Gruneisen parameter for materials with simple lattice was obtained:

$$\Gamma = -\frac{\sum\limits_\beta \left((d+2)\, \Phi'\left(a_\beta^2\right) a_\beta^2 + 2\Phi''\left(a_\beta^2\right) a_\beta^4 \right)}{d \sum\limits_\beta \left(d\Phi\left(a_\beta^2\right) + 2\Phi'\left(a_\beta^2\right) a_\beta^4 \right)}, \tag{12}$$

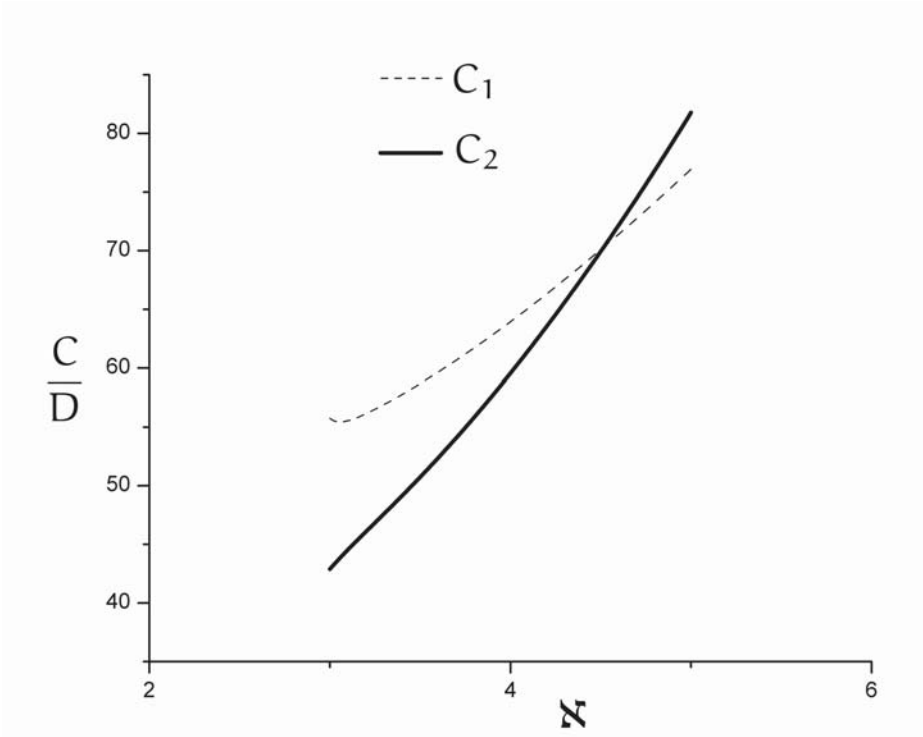

Figure 2: Dependence of stiffnesses on $\aleph$

where

$$\Phi\left(a_\beta^2\right) = -\frac{\Pi'(a_\beta)}{a_\beta}. \tag{13}$$

Using (12) and (13), one can obtain dependence of Γ on $\aleph$. This dependence $\Gamma(\aleph)$ is presented at fig 3. This dependence is monotonic. It means, that it can be unambiguously inverted. One can find dependence of ratio C_1/C_2 on Γ, graph for which is presented at the fig. 4. So, it is possible to find such a value Γ_*, that the BCC lattice is stable in view of $\Gamma < \Gamma_*$ and unstable in view of $\Gamma > \Gamma_*$. As it will be shown further in this paper, BCC lattice transforms to face-centered cubic (FCC) lattice when it becomes unstable. The Gruneisen parameter of material with FCC lattice is greater than one for material with BCC lattice and with the same α. That's why the stability condition can be rewrited in the following form:

$$\Gamma < \Gamma_* \cong 1.713 \tag{14}$$

This criterion was succesfully verified for more than 30 materials. Results for some of these materials, which are the closest to the boundary of stability, are presented in table 1. From the table 1 one can see when $\aleph$ is such, that BCC lattice is stable, the material always has BCC lattice, not FCC. It can be explained by the fact, that bonding energy for BCC lattice is higher than for FCC.

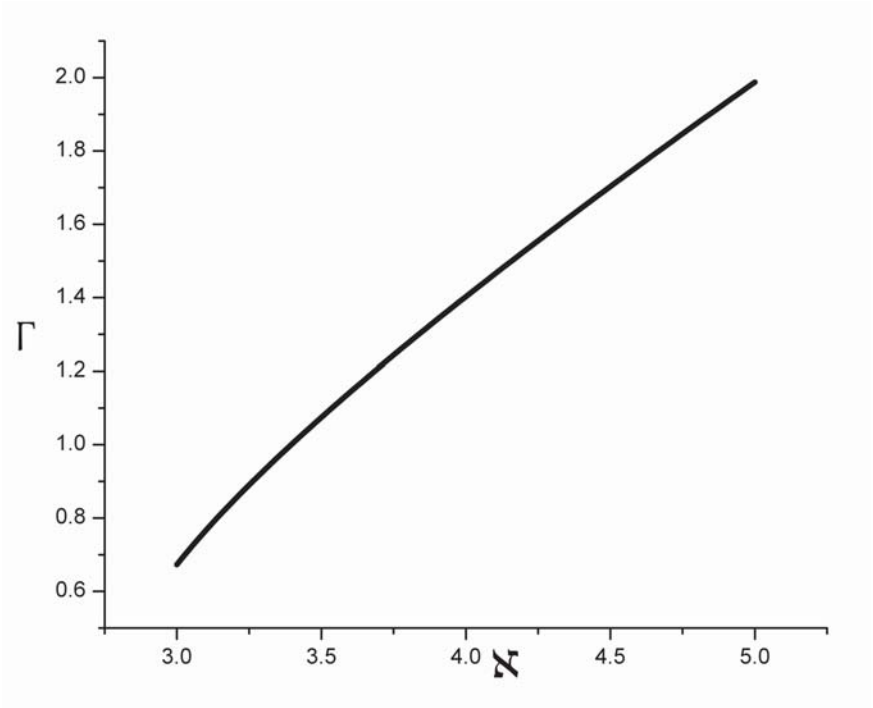

Figure 3: Dependence of Gruneisen parameter on א

Metall	Γ	Lattice
Molybdenum	1.58	BCC
Iron	1.68	BCC
Niobium	1.68	BCC
Tantalum	1.69	BCC
Nickel	1.91	FCC
Copper	2.04	FCC

Table 1: Gruneisen parameters for materials with different lattices

5 Numerical modelling

The loss of stability of BCC lattice was simulated in numerical experiment. Besides the interatomic interaction, described by potential (1) with א, corresponding to unstable lattice, small dissipation was introduced into the model. Particles had random velocities, in the range 0–0.1 v_0 (v_0 is the long-wave velocity). Method of central differences was used for integration. The step of integration was equal to 4% of the period of characteristic oscillations of the particles. The motions in the system became unapparent after time, equal to 120 periods of oscillations. The procedure of numerical integration is specified in [1].

The first result obtained was that criterion (11) is correct: the BCC lattice for material, satisfying (11) is stable and vice versa. The problem is to figure out to which lattice the BCC lattice transforms when it loses stability. To solve this problem the coordinational diagram was plotted. Coordinational diagram is a diagram, showing the quantities of atomic pairs with different interatomic distances. For

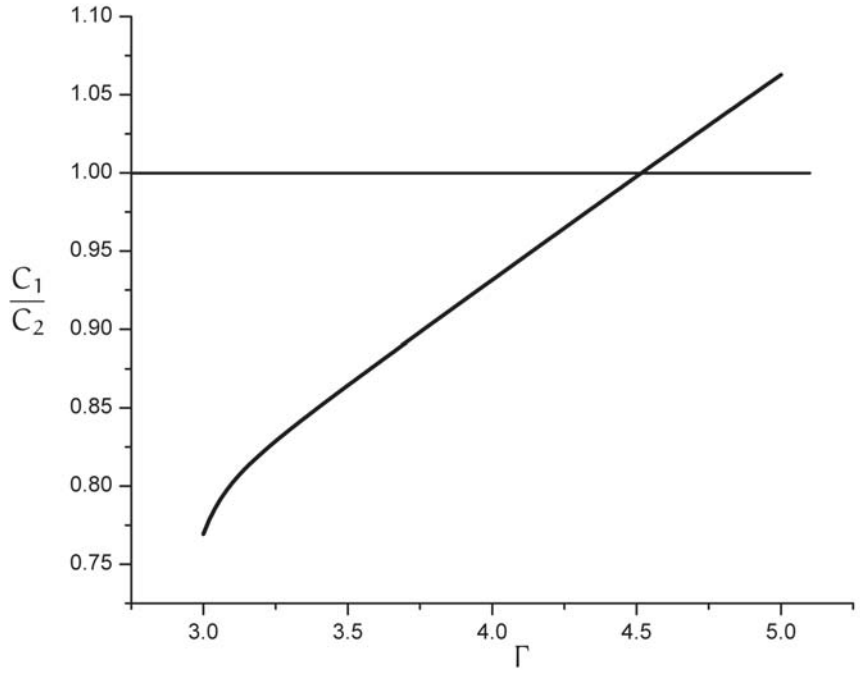

Figure 4: Dependence of ratio of stiffnesses on Γ

ideal BCC lattice this diagram looks as at fig. 5: it has several peaks, corresponding to radiuses of coordination spheres. The final coordinational diagram is shown at figure 6. The analysis of these diagrams gives several results. The first parameter analysed was the number of atoms in the first coordinational sphere (the number of the "closest" atoms, which is also called the coordinational number). This quantity was counted for all the atoms. At the beginning the coordinational number is equal to 8 for each atom. The coordinational number distribution after the destruction of the BCC lattice can be seen in the table 2. As one can see, the majority of the atoms has the coordinational number 12 after the structural transition. This coordinational number corresponds to two FCC lattice. The ratios of radiuses of the first three coordinational spheres were counted to find out what the prevalent lattice is. Radius of the n-th coordinational sphere is equal to an absciss of the n-th maximum on a coordinational diagram. This ratios are presented in table 3. As

Coordinational number	Percent of atoms, having this coordinational number
6	1.4
7	3.4
8	2.4
9	3.1
10	7.2
11	17.9
12	63.8

Table 2: Coordinational number distribution of atoms.

one can see from table 3, the values after the transition are close to the FCC values.

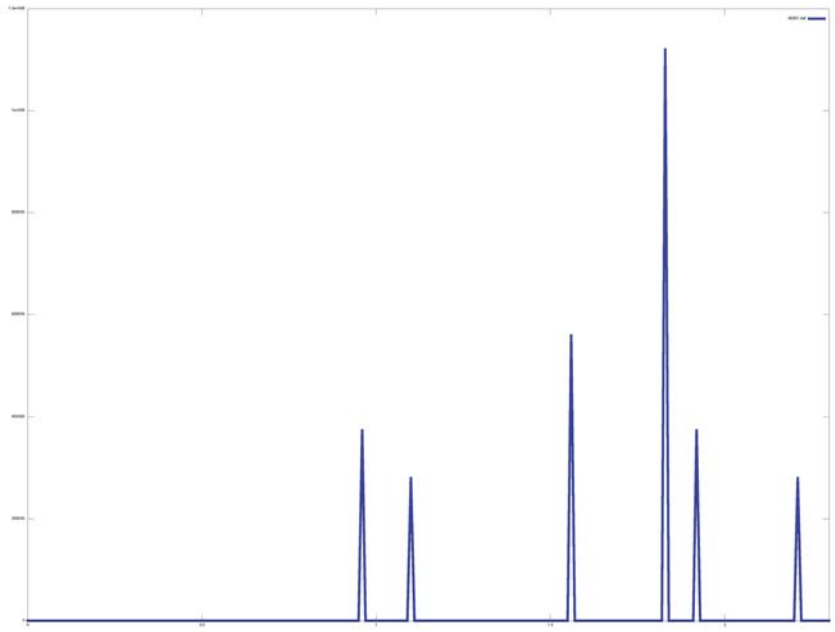

Figure 5: coordinational diagram before destruction of the BCC lattice

	BCC lattice	FCC lattice	Before transition	After transition
r_2/r_1	1.15	1.41	1.15	1.41
r_3/r_1	1.64	1.73	1.64	1.73

Table 3: Ratios of radiuses of coordinational spheres

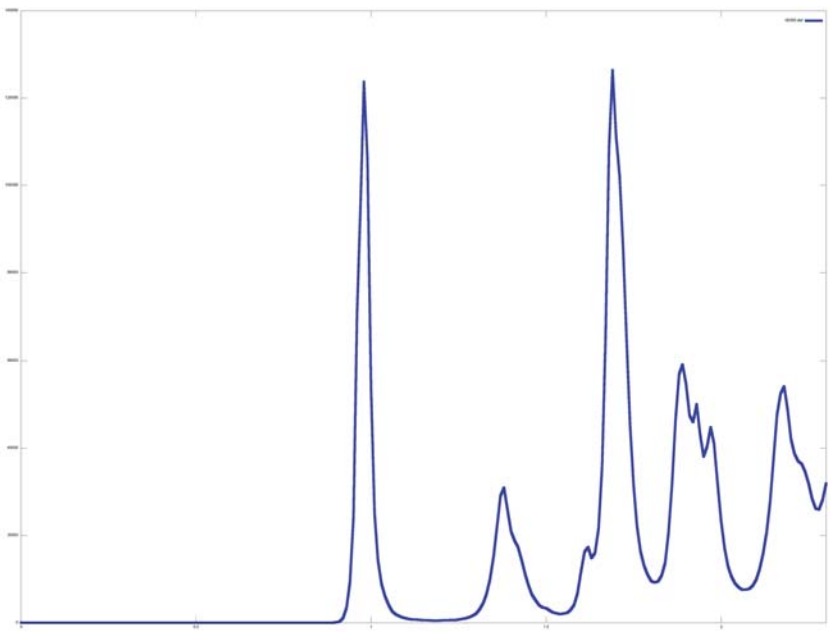

Figure 6: coordinational diagram after the destruction of the BCC lattice

So, it allows us to expect the BCC to FCC structural transition. The ratio $\frac{r_2}{r_1}$ for the atoms, which have the coordinational number 8 is equal to 1.41. So, the rest of atoms is not BCC. It was noticed, that after the transition the Gruneisen parameter raised: before the transition it was equal to 2.61 and after it became equal to 2.69. It means, that the increase of the Gruneisen parameter, predicted analytically takes place in the numerical experiment. It gives hope to be able to simulate such phenomena as the phase transition from BCC to FCC lattice, which takes place in iron.

6 Concluding remarks

In this paper the stability criterion for body-centered cubic lattice is obtained. This criterion was verified with the numerical simulation. It was also reformulated in terms of Gruneisen parameter. This reformulated criterion was verified by comparison with known experimental results. Both verifications showed the correctness of this criterion. The transition from unstable BCC to FCC lattice was modelled. Analogous modelling can be used to describe this transition, taking place with the raise of temperature in iron. As one can see from table 1, iron is the BCC metall, one of the closest to the instability region. It allows to expect loss of stability of BCC lattice under temperature raise, connected with predicted raise of Gruneisen parameter (it is condidered to be temperature independent in classical theories, but many investigations [6], [7] showed, that it is not).

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