

# Influence of defects distribution and specimen size on fracture initiation

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## Abstract

An analytical model for the scale dependence of the fracture initiation is suggested. The model is based on the idea that fracture is a stochastic process, for the bigger specimens probability of joint defects is higher, and this stimulates the fracture. An analytical formula for the strength dependence on the specimen size and defects density was obtained and compared with the molecular dynamics simulation. The results show that generally there is no similarity in fracture of the specimens of the different size and scale. This also prevents from using representative volume for the material strength properties.

## 1 Introduction

The defect structure of material has essential and sometimes unexpected influence on the strength properties. One of such results [1] is shown in Fig. 1. The figure is obtained by MD (molecular dynamics) simulation of cyclic loading of monocrystal material with randomly distributed defects (vacancies). The density of defects for the specimen in Fig. 1a is 10 times lower then for the specimen in Fig. 1b. The

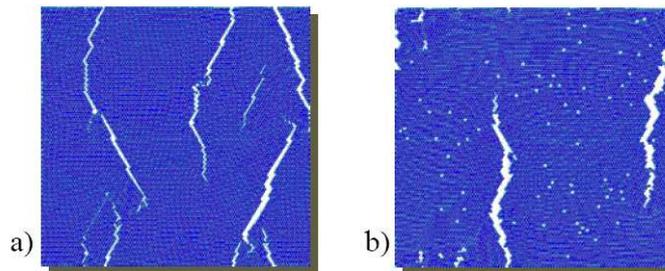


Figure 1: Crack development in crystals: a) 0.1% defects; b) 1.0% defects.

unexpected result is that for the lower density of defects the number of cracks is higher. The explanation of this fact is that for the higher density of defects the crystal contains occasional zones where the defects are very close to each other — these zones initiate the cracks — see Fig. 2. For the lower defects density all vacancies

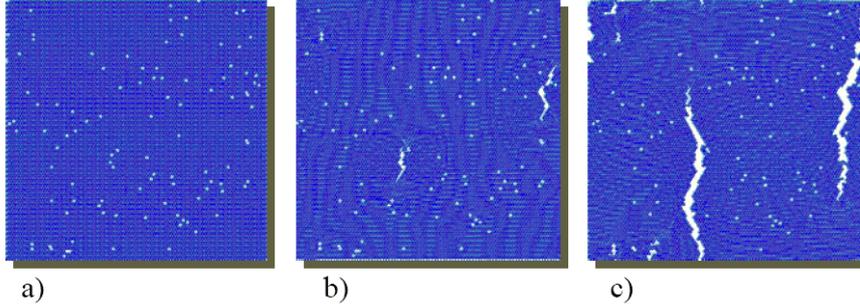


Figure 2: Crack development in crystal with 1% defects

are separated and all of them initiate cracks. Of course, the material strength in the last case is much higher. However this result can be changed if the bigger specimens would be observed, then even for the low defects density the probability of two defects to appear closely to each other could be high enough, and then they would produce the weak zones in which crack would initiate. Thus, the fracture scenario can differ for specimens of different sizes, even if the defects density is equal. The current paper is mainly devoted to study of such phenomenon. Below, an analytical model for the analysis of the scale dependence of the material strength is suggested and compared with the results of MD simulation.

## 2 Analytical model

Let us consider an ideal crystal, containing randomly distributed defects — vacancies. Each vacancy is formed by removing a single atom from the lattice. The material is weaker in the places, where the vacancies are close to each other. The most dangerous situation is when two vacancies are formed from the neighboring atoms — this structure we will call double vacancy. Let us calculate the probability of formation of the double vacancy.

Let the crystal contain  $N$  atoms, each atom has  $M$  neighbors. For closed packed lattices  $M = 6$  in 2D and  $M = 12$  in 3D. Let us remove sequentially atoms from the lattice to form vacancies. The probability that a double vacancy will appear after  $n$  atoms are removed will be denoted as  $\xi_n$ . Then the following recurrent relation fulfils

$$\xi_{n+1} = \xi_n + (1 - \xi_n) \frac{Mn}{N}. \quad (1)$$

Indeed, the first term  $\xi_n$  in the above relation gives the probability that the double vacancy was formed at the step  $n$ , the probability of the otherwise is  $1 - \xi_n$ . Then, the probability that in this situation the new vacancy number  $n + 1$  will appear near one of the previous vacancies is proportional to the number  $Mn$  of atoms neighboring to vacancies, divided by the total number of atoms  $N$ . To obtain relation (1) it was assumed that the density of vacancies is low:  $n \ll N$ . This assumption allows us to neglect the situation when one atom is a neighbor for two vacancies, and also we neglect that the total number of atoms is decreasing. The mentioned approximations little bit increase both numerator and denominator in relation (1), therefore together

this effects should not give a considerable error. Relation (1) can be rewritten in the form

$$\zeta_{n+1} = (1 - \varepsilon n) \zeta_n; \quad \zeta_n \stackrel{\text{def}}{=} 1 - \xi_n, \quad \varepsilon \stackrel{\text{def}}{=} M/N. \quad (2)$$

Here  $\zeta_n$  is the probability that a pair of double vacancies will NOT appear after  $n$  atoms are removed;  $\varepsilon$  is a small parameter; for any  $n$  fulfills:  $\varepsilon n < 1$ . Since  $\zeta_1 \equiv 1$ , from the recurrent relation (2) it follows

$$\zeta_{n+1} = \prod_{k=1}^n (1 - \varepsilon k) \quad \Rightarrow \quad \ln \zeta_{n+1} = \sum_{k=1}^n \ln(1 - \varepsilon k). \quad (3)$$

Assuming that the number of vacancies is a big value:  $n \gg 1$ , the last sum can be calculated as

$$\ln \zeta_n \approx \ln \zeta_{n+1} = n \sum_{k=1}^n \ln \left( 1 - \varepsilon n \frac{k}{n} \right) \frac{1}{n} \approx n \int_0^1 \ln(1 - \varepsilon n x) dx. \quad (4)$$

Calculation of the integral gives

$$\ln \zeta_n = -\frac{1}{\varepsilon} (1 - \varepsilon n) \ln(1 - \varepsilon n) - n \quad \Rightarrow \quad \zeta_n = e^{-n} (1 - \varepsilon n)^{-(1-\varepsilon n)/\varepsilon}. \quad (5)$$

Let us consider

$$\varepsilon n = \frac{Mn}{N} = Mp, \quad p \stackrel{\text{def}}{=} \frac{n}{N}. \quad (6)$$

Here  $p$  is porosity. It was already assumed that porosity is small:  $p = n/N \ll 1$ . For simplification of formula (5) let us assume that  $\varepsilon n = Mp \ll 1$ . Please note that this assumption gives more strict constriction for the smallness of  $p$ , since  $M$  is of order of 10. Anyway, for  $\varepsilon n \ll 1$  in the first nontrivial approximation from (5) we obtain<sup>1</sup>

$$\ln \zeta_n = -\frac{1}{2} \varepsilon n^2 \quad \Rightarrow \quad \zeta_n = e^{-\frac{1}{2} \varepsilon n^2}. \quad (7)$$

For the further consideration let us change parameters  $\varepsilon, n$  to parameters  $p, N$  using formulae

$$n = Np, \quad \varepsilon = \frac{M}{N}; \quad \varepsilon n = Mp, \quad \varepsilon n^2 = MNp^2. \quad (8)$$

Parameters  $\varepsilon, n$  were more convenient for calculations, however parameters  $p, N$  have more clear physical meaning — porosity and total number of particles. Then probability  $\xi_n = 1 - \zeta_n$  of the double vacancies appearance can be represented as a function of these quantities:

$$\begin{aligned} \xi(p, N) &= 1 - e^{-n} (1 - Mp)^{-(1-Mp)N/M}, & p \ll 1; \\ \xi(p, N) &= 1 - e^{-\frac{1}{2} MNp^2}, & p \ll \frac{1}{M}; \\ \xi(p, N) &= \frac{1}{2} MNp^2, & p \ll \sqrt{\frac{2}{MN}}. \end{aligned} \quad (9)$$

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<sup>1</sup>For correct result the two-term expansion for  $\ln(1 - \varepsilon n)$  is required.

At the left side of each formula the corresponding restriction for the porosity is given. For the first formula this restriction is the weakest. For the second formula it is little bit stronger, however the formula is much simpler. Since the difference in the restrictions is small, then for most cases the second formula can be used instead of the first one; it will be shown later that the error in this case is even less than can be expected. For the last formula in (9) the corresponding restriction is very strong. Thus the last formula is valid only for very low porosity, moreover the bigger is the specimen, the lower should be the porosity. However the last formula has the simplest form and can be easily analyzed. From this formula it follows that the probability for the double vacancy is proportional to the square of porosity and to the total number of particles. The last fact is very important — it means, that specimens of different size can have different mechanisms for fracture. Indeed, if the specimen is small enough, then appearance of joint vacancies is unlikely, and the fracture will be initiated from single vacancies. The bigger specimens are likely to have double vacancies — since the fracture will be initiated from them, and this requires much lower stresses, than for the single vacancies in the small specimens. Thus there will be no similarity in fracture of the specimens of the different size and scale. This also means that the representative volume for the material strength properties does not exist. These conclusions follow directly from the third formula in (9), however the first or second formulae from (9) (more exact approximations) lead to the same conclusions — the probability for the double vacancies essentially depends on the total number of particles  $N$ .

Let us rewrite the third formula from (9):

$$\xi(p, N) = \frac{1}{2} MNp^2, \quad p \ll \sqrt{\frac{2}{MN}}. \quad (10)$$

This formula can be also used to estimate the density of the double vacancies in material. If we consider that the material is combination of  $N_s \gg 1$  specimens with  $N$  particles each, then the number of double vacancies  $n_2$  in such material can be calculated as

$$n_2 = N_s \xi(p, N), \quad p_2 \stackrel{\text{def}}{=} \frac{n_2}{N_s N}. \quad (11)$$

Here  $p_2$  — is the density of double vacancies in the material. Substituting the above relations to the last formula in (9) we obtain

$$p_2 = \frac{1}{2} Mp^2, \quad p \ll \frac{1}{M}. \quad (12)$$

Thus the density of the double vacancies is proportional to the square of porosity. The restriction  $p \ll 1/M$  was taken from the second formula in (9). Let us show that if the material contains enough particles then it can be divided in specimens with  $N$  particles each, so that restriction from (10) will be fulfilled. Using restriction for formula (10) we can obtain inequality for the number of particles in the specimen

$$M \ll N \ll \frac{2}{Mp^2} \Rightarrow p \ll \frac{\sqrt{2}}{M}. \quad (13)$$

The obtained inequality for porosity guarantee that the material can be divided in specimens containing enough particles to use formula (10). But this inequality is weaker than  $p \ll 1/M$ , therefore it is already fulfilled.

Let us apply the obtained results for estimation of the strength properties of a specimen with  $N$  particles and porosity  $p$ . Let  $\varepsilon_1$  and  $\varepsilon_2$  be the critical strains for the fracture initiation from a single vacancy and a double vacancy. Then the critical strain for the specimen can be estimated as

$$\varepsilon(p, N) = \varepsilon_1 \zeta(p, N) + \varepsilon_2 \xi(p, N) = \varepsilon_1 + (\varepsilon_2 - \varepsilon_1) \xi(p, N). \quad (14)$$

The same formula can be written for other critical parameters, e. g. ultimate strength. Using formula (14) we consider fracture as a stochastic process, therefore strength properties should be obtained as average over many tests. When deriving equation (14) we have used the following rude assumptions:

1. Vacancies interact only when they are joined.
2. Junction of more than two vacancies does not exist.

Of course these assumptions are not completely true, especially the first one. However they allow to estimate the dependence of material properties on the porosity and the specimen size, as it will be shown in the next section.

### 3 Computational model

The simulation procedure applied in this work is conventional MD technique, same as in [2], in more details it is described in [3, 4]. The material is represented by a set of particles interacting through a pair potential  $\Pi(r)$ . The equations of particle motion have the form

$$m \ddot{\underline{r}}_k = \sum_{n=1}^N \frac{f(|\underline{r}_k - \underline{r}_n|)}{|\underline{r}_k - \underline{r}_n|} (\underline{r}_k - \underline{r}_n), \quad (15)$$

where  $\underline{r}_k$  is the radius vector of the  $k$ -th particle,  $m$  is the particle mass,  $N$  is the total number of particles, and  $f(r) = -\Pi'(r)$  is the interparticle interaction force. We use the following notation:  $a$  is the equilibrium distance between two particles ( $f(a) = 0$ ),  $D = |\Pi(a)|$  is binding energy,  $C$  is the stiffness of the interatomic bond in equilibrium, and  $T_0$  is the period of vibrations of the mass  $m$  under the action of a linear force with stiffness  $C$

$$C = -\Pi''(a) \equiv -f'(a), \quad T_0 = 2\pi\sqrt{m/C}. \quad (16)$$

We will use the quantities  $a$  and  $T_0$  as microscopic distance and time scales. For a particle of mass  $m$  that is in equilibrium in the potential field  $\Pi(r)$  its minimum velocity to reach infinity is  $v_d = \sqrt{2D/m}$  — so called dissociation velocity. We will use this quantity as a velocity scale. To measure the level of thermal motion in material the velocities deviation  $\Delta v$  (mean-square value of random velocities) will be used. When  $\Delta v$  approaches dissociation velocity  $v_d$  then the thermal motion break the internal bonds in the material resulting in its melting.

Let us consider the classical Lennard–Jones potential:

$$\Pi_{LJ}(r) = D \left[ \left(\frac{a}{r}\right)^{12} - 2 \left(\frac{a}{r}\right)^6 \right], \quad (17)$$

where  $D$  and  $a$  are the binding energy and the equilibrium interatomic distances, introduced earlier. The corresponding interaction force  $f(r) = -\Pi'(r)$  has the form

$$f_{LJ}(r) = \frac{12D}{a} \left[ \left( \frac{a}{r} \right)^{13} - \left( \frac{a}{r} \right)^7 \right]. \quad (18)$$

In the case of the Lennard–Jones potential, the stiffness  $C$  and the binding energy  $D$  obey the relation  $C = 72D/a^2$ ; the force (18) reaches its minimum value (the bond strength) at  $r = b = \sqrt[6]{13/7}a$ , where  $b$  is the break distance. The corresponding break deformation of the Lennard–Jones bond is  $\varepsilon_* = b - a \approx 0.109$ . The Lennard–Jones potential is the simplest potential that allows one to take into account the general properties of interatomic interaction: repulsion of particles that approach each other, attraction of particles moving away from each other, and the absence of interaction at large distances between them. For calculations the shortened Lennard–Jones interaction will be used, given by formula

$$f(r) = \begin{cases} f_{LJ}(r), & 0 < r \leq b, \\ k(r)f_{LJ}(r), & b < r \leq a_{\text{cut}}; \end{cases} \quad (19)$$

where  $b$  is break distance for Lennard–Jones potential,  $a_{\text{cut}}$  is cut-off distance (for  $r > a_{\text{cut}}$  the interaction vanishes). The coefficient  $k(r)$  is the shape function

$$k(r) = \left[ 1 - \left( \frac{r^2 - b^2}{a_{\text{cut}}^2 - b^2} \right)^2 \right]^2. \quad (20)$$

The cut-off distance will be set as  $a_{\text{cut}} = 1.4a$ , in this case only the first neighbors are interacting for the close-packed structures. In the current paper we study the fracture process in general, therefore, the proposed simplified potential is sufficient. The obtained results can be easily extended to more complex potentials describing the properties of materials more exactly.

In this work, a two-dimensional material will be used, where particles are packed to form an ideal 2D close-packed (triangular) crystal lattice. This is simplified lattice, however its symmetry is same as the symmetry of [111] cross-sections and surfaces of such 3D crystal lattices as FCC and diamond (the last one is the lattice of silicon crystals). For computations square specimens are used, periodic boundary conditions are applied at all boundaries. All specimens are subjected to uniaxial loading by applying a small uniform deformation to positions of all particles and to the periodic boundaries, after each step of deformation a step of MD computation is used. The deformation is changing according the formula

$$\varepsilon(t) = \varepsilon_{\text{max}} \frac{t}{t_{\text{max}}}, \quad (21)$$

where  $\varepsilon_{\text{max}}$  is the maximum value of strain,  $t_{\text{max}}$  is the time of computation. The strain is directed along one of the sides of triangles, forming the lattice. The computation parameters are given in the Table 1.

Parameter	Symbol	Value
Number of particles	$N$	$10^4 \div 10^5$
Porosity	$p$	$10^{-4} \div 10^{-2}$
Cut-off radius	$a_{\text{cut}}$	$1.4 a_0$
Initial velocity deviation	$\Delta v$	$0.005 v_d$
Integration step	$\Delta t$	$0.02 T_0$
Calculation time	$t_{\text{max}}$	$50 T_0$
Maximum strain	$\varepsilon_{\text{max}}$	0.1

Table 1: Computation parameters.

## 4 Results of computations

Fig. 3a shows dependencies of the critical strain on porosity obtained from the computer experiments. Two sizes of specimens are considered:  $N = 10\,000$  and  $N = 100\,000$ . The same graphs obtained analytically using estimation (14) are

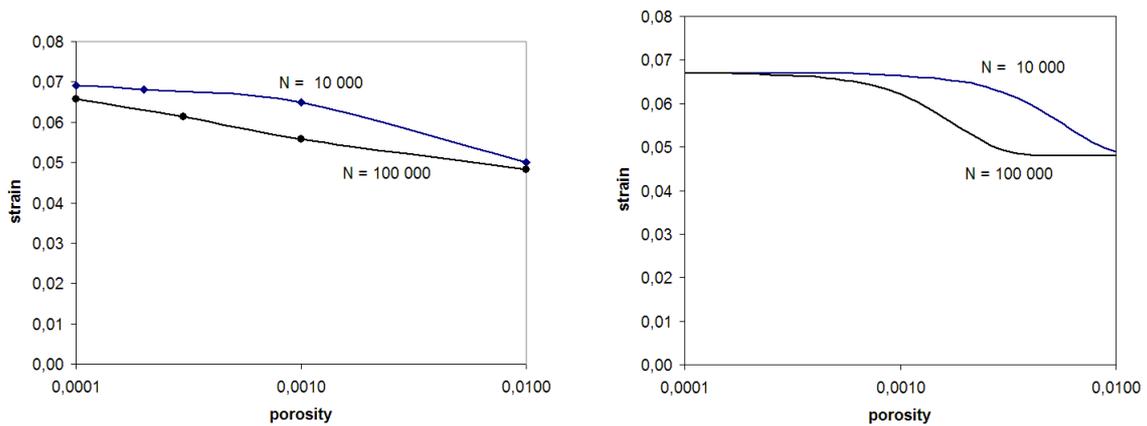


Figure 3: Comparison of results for different sizes of specimens: a) MD computations, b) analytical model.

shown in Fig. 3b. To obtain these graphs first or second formula from (9) can be used, the difference between them is negligible<sup>2</sup>. The values of the parameters used for the analytical calculations are

$$\varepsilon_1 = 0.067, \quad \varepsilon_2 = 0.048; \quad M = 6. \quad (22)$$

Results of the both models, MD and analytical, show the same tendencies: the strength of the bigger specimen is considerably lower, then for the smaller one; the scale effect is smaller for high and low porosities, and it has maximum for the intermediate porosities. The explanation for the last fact is that for low and high porosities both specimens have the similar mechanism for the fracture initiation:

<sup>2</sup>The maximum difference between the first and the second formula from (9) while calculating graphs Fig. 3a is lower then 1% for  $\xi(p, N)$  calculation and lower then 0.2% for the critical strain calculation.

single vacancies for low porosity and double vacancies for high porosity. In the case of intermediate porosity the situation is scale-dependant, because the smaller specimen is unlikely to have double vacancies in this case, but for the bigger specimen the double vacancies are much more probable.

Thus, qualitatively computational and analytical graphs are similar, but quantitatively they have differences: the computational graphs are more flat, and the maximum scale effect appears at different porosities. Fig. 4a,b shows comparison of computational and analytical models for the small and big specimen respectively.

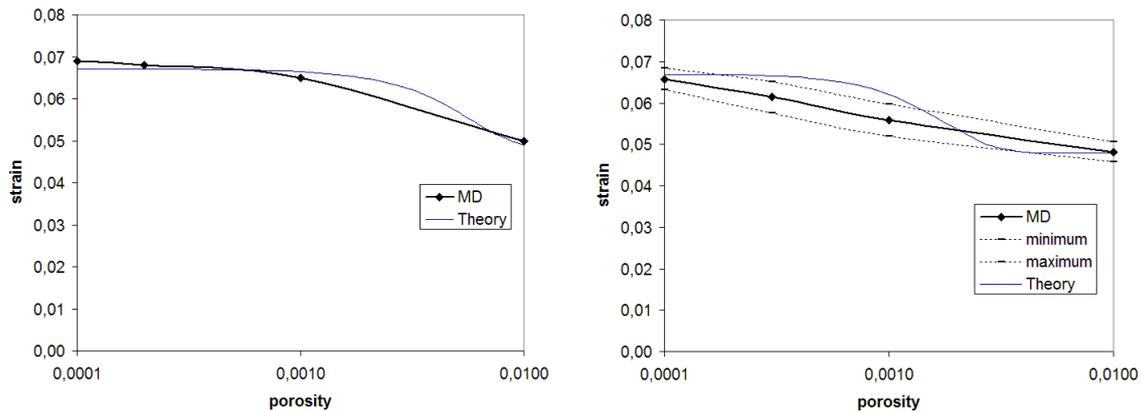


Figure 4: Comparison of results of MD computer experiments and predictions of analytical model: a)  $N = 10\,000$ , b)  $N = 100\,000$ .

In Fig. 4b together with the average computational result an error corridor obtained for the series of 5 experiments is shown. The theoretical curve gets inside the error corridor for the low and high porosities, but escapes from it for the intermediate porosities. The main explanation for the differences between the computational and analytical models is that the assumption that vacancies interact only when they are joined is too rude. Of course two closely located vacancies interact and such place is likely for fracture initiation. This effect can be also described analytically by the similar method as it was used above for the double vacancies, but such description requires additional calculations and also an estimation of the influence of the distance between the vacancies on the critical strain. For the bigger specimens also appearance of more then two joint vacancies should be taken into account.

## 5 Conclusions

An analytical model for the scale dependence of the fracture initiation is suggested. The model is based on the idea that fracture is a stochastic process, for the bigger specimens probability of joint defects is higher, and this decreases the material strength. Thus there is no similarity in fracture of the specimens of the different size and scale. This also means that the representative volume for the material strength properties does not exist. Indeed, the bigger is the specimen, the more sophisticated joining of defects can appear in it, giving new mechanisms for the fracture initiation.

The probability for double vacancies was calculated, and the material strength properties as a function of defects density and specimen size were estimated. These results were compared with MD simulations. Results of both models, MD and analytical, show the same tendencies: the strength of the bigger specimen is considerably lower than for the smaller one; the scale effect is smaller for high and low porosities, and it has maximum for the intermediate porosities.

Qualitatively computational and analytical graphs are similar, but quantitatively they have differences: the computational graphs are more flat, and the maximum scale effect appears at different porosities. The explanation for the differences between the computational and analytical models is that the assumption that vacancies interact only when they are joined is too rude, interaction of non-joined vacancies should be taken into account. This effect can be also described analytically by the similar method as it was used in the report for the double vacancies, but such description requires additional calculations and also an estimation of the influence of the distance between the vacancies on the critical strain. For the bigger specimens also appearance of more than two joint vacancies should be taken into account.

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## References

- [1] A. M. Krivtsov. MD modeling of low-cycle high-amplitude loading of monocrystal material with defects. Proc. of XXXIII Summer School “Advanced Problems in Mechanics 2005”, St. Petersburg, Russia, 2006, 341-346.
- [2] A. M. Krivtsov. Molecular dynamics simulation of plastic effects upon spalling. Phys. Solid State **46**, 6 (2004).
- [3] Allen M.P. and Tildesley A.K. Computer Simulation of Liquids. – Oxford: Clarendon Press. 1987. 385 .
- [4] A. M. Krivtsov. Deformation and fracture of solids with microstructure. Moscow, Fismatlit. 2007. 304 p. (In Russian).

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