# FRACTURE PROCESS UNDER TENSION DEFORMATION OBSERVING USING COMPUTER SIMULATION METHOD

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## ABSTRACT

Fracture process stages of crack-free solid Ar under tension deformation were observed at atomic scale using variational quasistatic method. The model had enough degrees of freedom to allow simulation of any kind of deformation and damage mechanisms. The atomic configuration, atomic displacement and local energy distribution can be monitored and plotted throughout at any steps computer record. From the atomic configuration and local energy distribution the fracture process divided in to five stages. The fracture stages were the following. The first stage was phase transition from homogeneous crystal to unhomogeneous by initiation of dislocations in a random direction throughout the crystal. On the second stage microvoids initiated and formed in different sizes at different positions. The third stage in fracture process was forming of mean crack from coalescence of microvoids and voids. At the forth stage the voids and microvoids were connected with the mean crack and leaded to crack growth. From the results of simulation, it was found that at final stage (end of relaxation process) the crystal was divided in two parts.

## INTRODUCTION

Many scientists have studied the problems of materials fracture during several centuries. They studied such problems in two main directions: experiment and attempts of theoretical basing. As a rule, experimental investigations require accumulation of definite statistics. Similar investigations demand the presence of investigating specimens of materials, which have identical characteristics, identity in carrying of each experiment, appears to be realised for monocrystal specimens partially.
Historically, main theories of fracture were based on the positions and ideas of entire medium mechanics, at present time the method of finite elements is applied at construction of fracture theory [1-3]. At the same time it was established, that structure-energetical processes, having place in material being under deformation at microscopic atomic level influence on mesomechanics of fracture. It is difficult to follow experimentally the realistion of similar processes, because in many cases they are realised in high speed, especially in cases of brittle fracture.
Developing methods of investigation of microscopic mechanics, based on computer experiment allowed to clear the whole series of important factors from the point view of physics and mechanics, regulating fracture processes at the atomic level, having place in the materiel. It is necessary to adequate presentation of the character of interatomic, intermolecular, long distance interaction in the computer experiment. Investigating crystal should contain enough quantity of atoms, molecules, in order the obtaining results could be spread from microscopic to higher levels: mesoscopic and macroscopic [4].
At present time two main approaches are developing in computer experiment [5-18]. They are methods of variational quasistatics and molecular dynamics. The second method shows clearly the dyunamics of fracture process taking into account such factors as time and temperature. But it is

necessary much time for the computer experiment, method of variational quasistatics solve the problem of structure energetical reconstruction, having place in the material by searching the minimum of crystal internal energy under deformation. The given method allows to find energetically advantages material structure at the atomic level, wasting not so much time.
Ductile fracture of solid under tension stress consists of number successive stages: phase transition from homogeneous to unhomogeneous, microvoids nucleation, formed a men crack from coalescence of microvoids and voids and finally a full fracture appeared [19].
The dynamics of fracture process in time, caused the accumulation of broken bonds between elements of the materials, depending on deformation and temperature is determined by following formula [18],

$$t = \psi \exp(-\gamma\sigma/K_B T) \quad \ldots\ldots 1$$

where t is the time of fracture, $\sigma$ is applied stress, $\psi$ and $\gamma$ are kinetic constants of material, $K_B$ is Boltzmann constant, T is temperature.
From this equation it was explained that the failure of the bonds is caused by the thermofluctuational process. In addition, the formation of microvoid is likely to be caused by the atomistic (theromofluctuational) process.
This paper describes the results of a computer simulation of fracture process stages in solid Ar.
The given paper is dedicated to the investigation of fracture process, taking place in crystal of solid Ar subjected to deformation of tension. Computer experiment was carried out by the method of variational quasistatics

## THE SIMULATION MODEL

It was used a developed variational quasistatic method to study the fracture phenomenon, the model was by Ovcharov et al described in previous publication [20-22]. In brief, the crystal considered in our work had FCC lattice and the crystal sample consisted of a set of hard monoaxial infinite chains with orientation <211>, and with three degrees of freedom. One was longitudinal and two were transversal components of displacement vector, thus the crystal was presented as a quasithree-dimensional and it looked like a set of rectangular nodes, each nod was presented as an atom. The number of atoms were 2400 atoms arranged in 24 rows along the X-axis and 100 atomic rows in the direction of the Z-axis, the Z-axis was directed along the infinite edge, the X-axis was perpendicular to the (101) plane and the Y-axis was perpendicular to (111) plane, the XOY undeformed crystal was presneted as in figure 1-a. It was chosen the sample of rare-gas solid Ar defining the model material to perform simulation. The Lennard-Jones (LJ) (6,12) pair potential is used for interatomic interaction between atoms with a solid Ar parameters in form:

$$\Phi_{ij}(r_{ij}) = 4\varepsilon_0 [(d/r_{ij})^{12} - (d/r_{ij})^{6}], \quad \ldots\ldots 2$$

where d is equilibrium distance between the nearest pair of atoms, corresponded to minimum energy of the bond, $r_{ij}$ is the distance between arbitrary pair of atoms i and j. $\varepsilon_0$ is the depth of the energetic minimum of two atom interaction. The interaction radius was equal to 9-10 coordinational sphere length, i.e. each atom interacted with 164 neighbours. Periodic boundary conditions were used and it allowed the atoms to move in all the directions, the model had more freedom to allow simulation of any kind of deformation and damage mechanisms. Therefore the simulation results were more reliable. The tension deformation was applied to crystal in [111] direction and it was applied a small thermal disturbance. Then the crystal relaxed to minimum potential energy, as a result the transformation processes appeared in the crystal.
During the relaxation process at different Steps Computer Record (SCR) and at the end of it the atomic configuration, the atomic displacement sequences number of atoms and local energy distribution map were monitored and plotted throughout.

## THE SIMUALTION RESULTS AND DISCUSSION

It was discovered the first stage in fracture process of a crack-free crystal was phase transition from homogeneous crystal to unhomogeneous by initiation of dislocations by atomic displacement in a

random direction throughout the crystal, this phase transition was clearly observed when was SCR equal to 7 as it was detected from atomic configuration in figure 1-b. Also it can be seen twinning deformation mechanisms in the crystal, these mechanisms were obviously observed when we compared figures 1-a and b. Twinning deformations have been detected before dislocations initiation. The same results were received by [7, 8].

The second stage appeared when the SCR was equal to 50. From the atomic configuration in the figure 1-c it can be seen that numbers of microvoids and voids initiated and formed in different sizes at different positions.

The last two stages of ductile fracture developed after the ultimate stress has been attained in plastic metal. At the end of the second fracture stage, it is was noted that, in industrial copper which had a FCC lattice, central crack begin to form near particles of microinclusions in the lattice Cu by destruction of proper particles of microinclusions. In addition, voids in commercial copper were seen unusually clear but in the most cases it was difficult to detect voids even after fracture [23].

The physical mechanism of microvoid initiation can be explained by the theory of dislocations, gliding dislocations can stop at various obstacles, resulting in strong stress concentration often sufficient for initiation of a microvoid.

When the SCR increased to 150, the simulation result showed that many microvoids had been coalesced into voids which could propagate rapidly in the direction perpendicular to the tension axis.

The third stage in fracture process was formation of mean crack from coalescence of microvoids and voids when a SCR was equal to 300. At this stage the number of voids and microvoids decreased.

Analyses of the atomic configuration showed that nucleation of several dislocations types and some of them formed and propagated to the direction ± Z. Increasing of twinning deformations could be clearly observed from the atomic configuration at the third stage of fracture. In addition, the main crack appeared in the core of the tensioned crystal, which was due to the character distribution of stresses in deformed crystal.

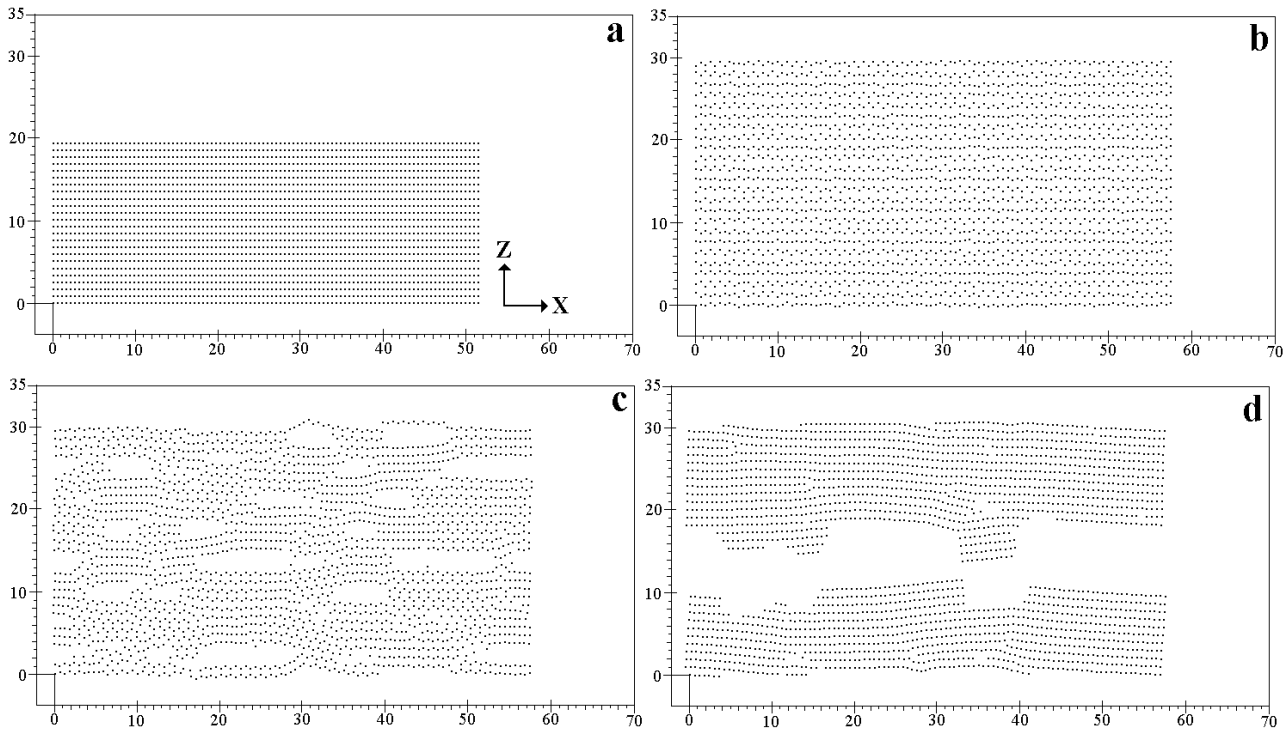


**Figure 1:** Atomic configuration: (a) the crystal model, (b) the simulation result at SCR equals to 7, (c) the simulation result at SCR equals to 50, (d) the simulation result at SCR equals to 800.

The forth stage appeared when the voids and microvoids joined to the mean crack and leaded to crack growth. The microvoids and voids decreased in number and in size. At the same time the twinning deformations increased when the SCR increased to 500.

When there were no large cracks in the body under loading, the microvoids formed randomly throughout the body and independently of one another. A full fracture took place at SCR 800 as it is shown in the figure 1-d. The twinning deformation increased to maximum as a full fracture appeared in the crystal.
From the results of simulation, it was found that the lattice was divided in two parts along the crystal. In addition, some dislocations formed and propagated to the crystal surfaces therefore the crystal surfaces were rough. It was assumed that, due to the crack growth, the number of microvoids and voids decreased to minimum till fracture appeared.
It can be seen from figure 1-d that the fracture line surfaces are rough and irregular. It can be suggested that the roughness observed on the fracture surface is simply the sign of very small crack branches, microcracks, which are smaller in size then the disturbance of process.
The Steps Computer Record (SCR) relaxation of potential energy in the crystal under tension deformation equal to the 34% is shown in figure 2. From figure 2 it can be seen that the energy needed to create the voids and microvoids in the second stage is much more then it is necessary for initiation of initial mean crack which needs more energy then it is necessary for growth and propagation.
It is interesting to note that in the dynamic studies the time-to-fracture with applied load is often used to determine the reliability and strength of materials. It was found that the first stage of fracture was the longest, first voids appeared, which joined into cracks and then at once followed the stage of fracture. The received results of sequence and duration of fracture correlates with experimental results, received at Al crystals by the authors [23].

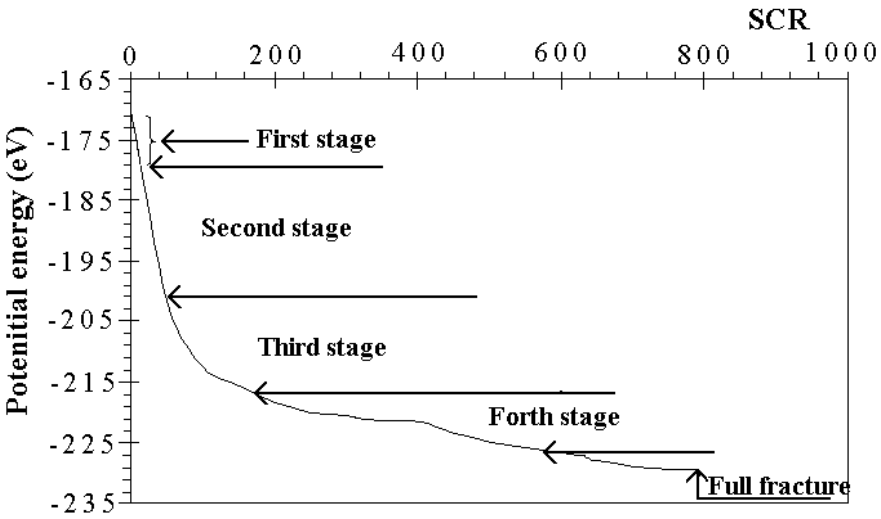


**Figure 2:** potential energy relaxation

When the crystal relaxed to minimum potential energy, the atoms moved from their location by different values of displacements corresponding to the interatomic potential between the atoms. The displacement sequences of number of atoms are shown in figures 3-a,b and c, where a is corresponded to SCR equal to 7, b at SCR to 50, c at SCR equals to 800.
The figures 3-a should be compared with 3-b, and c. From these figures we concluded that when SCR increased the number of atoms having a big displacement decreased. It happened because of the fact, that when SCR increased the initial crack formed from the coalescence of microvoids. In addition, the twinning deformations increased also. Thus the number of atoms having a big displacement decreased.

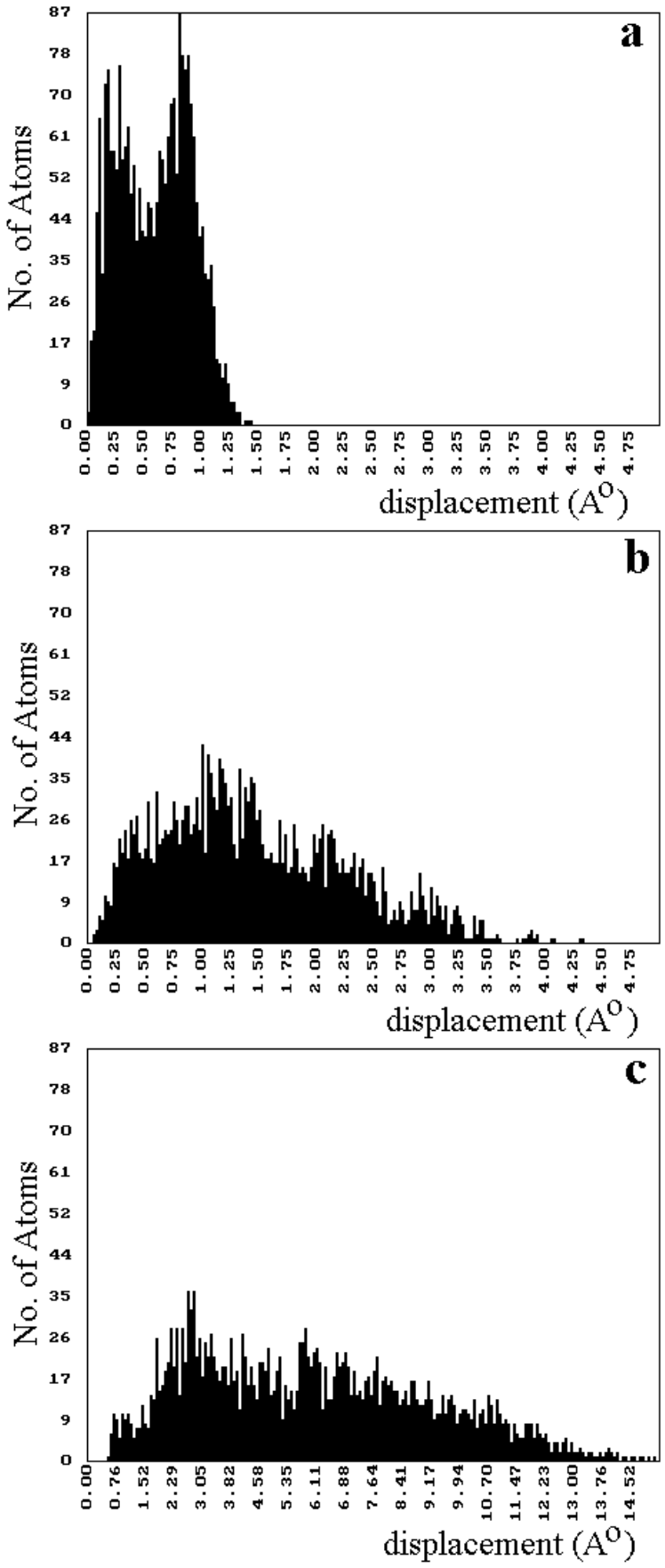


**Figure 3:** Sequence of number of atoms of displacement, (a) at SCR equals to 7, (b) at SCR equals to 50, (C) at SCR equals to 800.

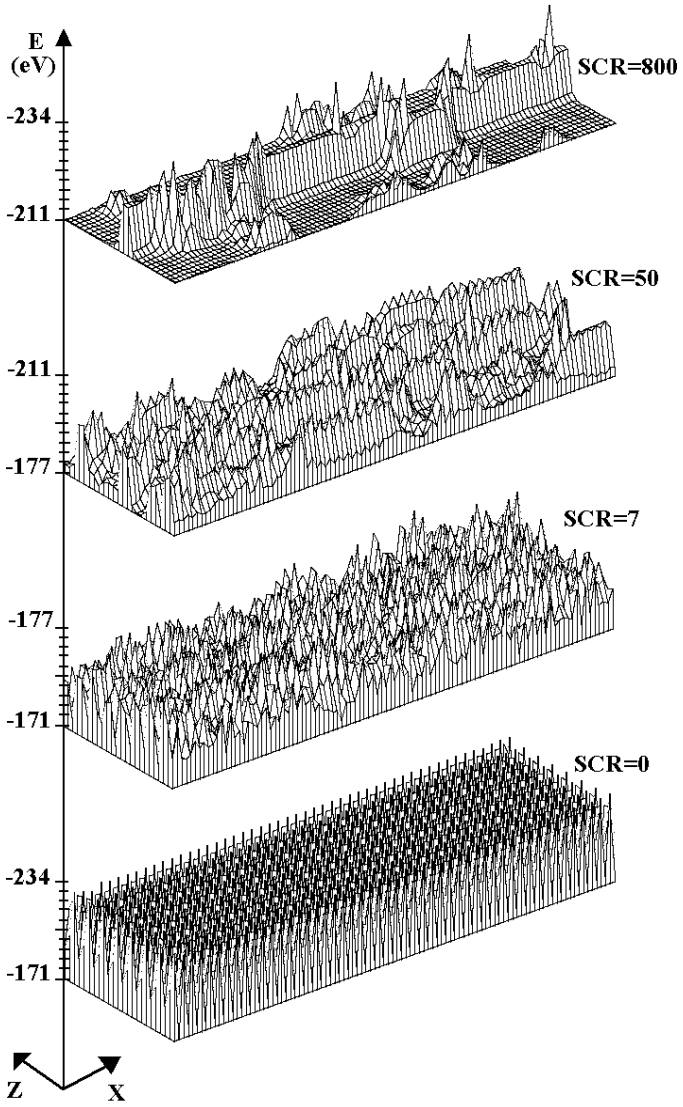


**Figure 4:** The local energy maps.

The stress of fracture for lattice with a rough surface can be raised by forming compressive stresses in the surface layer so as to prevent opening of surface cracks. This phenomenon is used for raising substantially the service life of metal parts by special methods of surface treatment: shot-blasting, roll forming and some procedures of heat treatment and chemical heat treatment [24].

Mishnaevsky et. al. [25] found that the surface roughness of the initial part of a crack and the surface energy needed to form a crack by the mechanisms of microcrack coalescence are much more then these values for the propagation crack.

It was found furthermore, that the fracture and features of the deformations had a close relation to the characteristic of energy distribution in the system [15]. We present the local energy distribution map figure at different SCR which can help to recognize all the stages, as it is shown in figure 4. Number of conclusions can be made concerning figure 4.

First, at zero SCR, all the atoms had the same potential energy and the energy map was uniform. Second, when SCR increased to 7, the local energy distribution map looked like not uniform, it was due to appearing of dislocations. The initiation of microvoids and voids stage was clearly observed in the energy local map when SCR increased to 7, the energy coalesced in different positions to initiated microvoids and voids. When SCR increased to 50 the mean crack initiated, which can be recognized from energy map. Finally the full fracture appeared when SCR was equal to 800 and was clearly observed in the energy map. In addition, the fracture line was in a zig-zag manner and the energy along the length of crack was not uniform in magnitude and fluctuated randomly.

Before the beginning of full fracture, a large values of local density of amount of potential energy stored in the elastic field of crystal.

It is worth to note that in the brittle fracture the sink was at the tip of crack where the stress field was high enough to separate atomic bonds creating new surface as the crack advances [24].
As we know, ductile fracture demonstrates large amounts of defects, thus the simulation results indicate, that the crack initiate and fracture is in ductile manner.
Macroscopically, ductile fracture surfaces have larger regions of crack and roughness of it's surfaces. Microscopically, ductile fracture surfaces also appear to be rough and irregular
Unfortunately there are not enough experiment data of peculiarities of solid Ar investigation. However, the presented results are in correspondence with experimental observation investigated by Ohr [26], using copper specimen under tension.

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