MD modeling of low-cycle high-amplitude loading of monocrystal material with defects

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Abstract

Fracture under low-cycle high-amplitude loading of 2D monocrystal material with predefined distribution of defects is studied using molecular dynamics technique. Influence of density of vacancies, lattice orientation, loading amplitude, loading period, thermal motion and interaction characteristics on the material strength, fracture process and crack topology are analyzed.

1 Introduction

Modeling of mechanical properties of MEMS require multiscale approach coupling continuum theories for creep and fatigue with discrete modeling based on atomic consideration and molecular dynamics simulation. The aim of this paper is to help constructing models of material behavior under cyclic mechanical loading by testing computational atomistic models of materials. The main point of interest is influence of material inner structure on its mechanical properties, crack propagation and resistance to cyclic loading.

In the last decades, the molecular dynamics (MD) method has been widely used to simulate deformation and fracture of solids [1–5]; the representation of a material as a set of interacting particles allows one to describe its mechanical properties at both micro and macrolevel [6, 7].

The mechanical properties of materials are rather sensitive to structural defects [8]. To take into account the influence of defects on material properties and describe the phenomena mentioned above we propose a model of a crystalline material with artificially introduced structural defects (vacancies).

2 Simulation procedure

The simulation procedure applied in this work is identical to that used in [5] and is described in details in [9]. The material is represented by a set of particles interacting through a pair potential $\Pi(r)$. The equations of particle motion have the form

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

where $r_k$ 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 $C$

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

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.
In this work, we analyze a two-dimensional material, 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). Let us consider the classical Lennard–Jones potential:

$$\Pi_{LJ}(r) = D \left( \frac{a}{r} \right)^{12} - 2 \left( \frac{a}{r} \right)^{6}$$ \hspace{1cm} (3)

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

$$f_{LJ}(r) = \frac{12D}{a} \left( \frac{a}{r} \right)^{13} - \left( \frac{a}{r} \right)^{7}$$ \hspace{1cm} (4)

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 (4) reaches its minimum value (the bond strength) at

$$r = b = \frac{\sqrt[3]{13}}{\sqrt{7}},$$

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 we will consider modification of the Lennard–Jones interaction, set by formula

$$f(r) = \begin{cases} f_{LJ}(r), & 0 < r \leq b, \\ k(r)f_{LJ}(r), & b < r \leq a_{cut}; \end{cases} \hspace{1cm} (5)$$

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

$$k(r) = (1 + \alpha) \left[ 1 - \left( 1 + \sqrt{\frac{\alpha}{1 + \alpha}} \right) \left( \frac{r^2 - b^2}{a_{cut}^2 - b^2} \right)^2 \right] - \alpha, \hspace{1cm} (6)$$

where $\alpha$ is positive parameter, defining brittleness of the material. Increase of $\alpha$ results in the repulsion appearing in the vicinity of the cut-off distance. This produces potential barrier for joining two particles, which where separated due to the material fracture. According to its definition the modified interaction coincides with Lennard–Jones one up to the break distance; this means that the main interaction parameters such as stiffness and bond strength are kept the same. For $\alpha = 0$ there is no potential barrier and formulae (5)- (6) simply give the shortened Lennard–Jones interaction, this variant of interaction we will use for most computations. The cut-off distance will be set as $a_{cut} = 1.4a$, in this case only the first neighbors are interacting for the close-packed structures. This simplifies comparison with analytical considerations, where only the first neighbors are taken into account and also allows to speed-up the calculations. In the current paper we study the principal possibility of describing the fracture under cycling loading rather than simulate the behavior of a certain material; therefore, the proposed simplified potentials are sufficient. The obtained results can be easily extended to more complex potentials describing the properties of materials more exactly.

3 Simulation of fracture

Let us consider an ideal crystal with a single defect (vacancy) — Fig.1a. The crystal is subjected to cyclic uniaxial tension:

$$\varepsilon_x = \frac{1}{4} \varepsilon_{\text{max}} \left( 3 - \cos \left( \frac{2\pi t}{T} \right) \right), \quad \varepsilon_y = 0, \hspace{1cm} (7)$$

where $\varepsilon_x$ and $\varepsilon_y$ are deformations along $x$ and $y$ axis (see Fig.1), $T$ is the period of loading. According to formula (7) the deformation is oscillating in the range: $\varepsilon_{\text{max}}/2 \leq \varepsilon_x \leq \varepsilon_{\text{max}}$. The maximum value $\varepsilon_{\text{max}}$ is chosen to be somewhat higher then the critical deformation for the crack initiation, $\varepsilon_{\text{max}} = 0.12$, $T = 10T_0$. The orientation of the lattice is vertical (the triangles are orientated vertically — see Fig.1). Here and below periodic boundary conditions are used at all boundaries. Due to anisotropy of the crystal four cracks are starting from the vacancy in four symmetrical crystallographic directions — Fig.1b. The further propagation of cracks can be seen in Fig.1c.
If the lattice is orientated horizontally, then the crack initiation scenario differs substantially — see Fig. 2. At first, the four cracks in crystallographic directions start from the vacancy (Fig. 2b) similar to the previous case. However, later on the cracks are turning towards alternative crystallographic directions. For some time the crack is propagating in the new direction and then turns again and again. At each turn dislocations start from the turning point, collisions of these dislocations produce new localized cracks, which can be seen in the outer areas of the specimen.

Now let us consider the crack initiation in the specimen with random distribution of vacancies — Fig. 3. The specimen has vertical lattice, the defects density is 1%, the number of particles is $10^4$, the deformation is cyclic and applied in the horizontal direction, the maximum deformation is $\varepsilon_{\text{max}} = 0.06$, the loading period is $T = 5T_0$. Fig. 3a shows the initial distribution of defects, Fig. 3b — the crack initiation, Fig. 3c — the developed cracks. An interesting effect is seen in Fig. 4d: after some time one of the cracks start to dominate over another one.

Comparison of crack development in different models of crystals is shown in Fig. 4. The cracks in the crystal, considered above are shown in Fig. 4b. For comparison in Fig. 4a the cracks in the crystal with 10 times lower density
of defects is shown. The 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.3b. For the lower defects density all vacancies
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 the probability of two defects to appear
closely to each other would be higher, and then they would produce the weak zones in which crack would initiate.

Fig.4c shows cracks in the material with 1.0% of defects but with modified law (5)–(6) of particles interaction with
\( \alpha = 2 \). The modification is aimed to make the material more brittle, this is made by adding small repulsion zone
after the point where the normal interaction force vanishes. This prevents particle bonds to be restored after they were
broken. The result is much higher density of cracks then for the ordinary interaction.

The effect of the lattice orientation on the crack development is shown in Fig.5. Much bigger specimens, containing
\( 10^5 \) particles are considered. The initial density of defects is 0.1%. According to the figure the vertical lattice produce
more regular cracks, and fracture in the horizontal lattice results in irregular cracks with frequent turning and bunching.

Graphs in Fig.5 show dependence of the critical deformation on the period of loading. The critical deformation
was obtained as minimum value of \( \varepsilon_{\text{max}} \) in formula (5) required to start fracture. Three specimens were tested for
\( 0 \leq t \leq 5T_0 \): 1) specimen from Fig.1 with single vacancy and vertical lattice; 2) specimen from Fig.2 with single
vacancy and horizontal lattice; 3) specimen from Fig.3 with 1% of vacancies and vertical lattice. For all specimens
it was obtained that the critical deformation is decreasing with the period increase. This coincides well with the
phenomenon of increasing material strength with the speed of deformation [10]. However sensitivity to the period of
loading for these specimens is different. The greatest effect is observed for the single vacancy in the vertical lattice
— the critical deformation drops in 20% when the period of loading is increased from \( 5T_0 \) to \( 20T_0 \). For the other two
specimens the critical deformation change is around 10%.

The highest value of the critical deformation for the single vacancies obtained for \( T = 5T_0 \) is about 74% of the
break deformation $\varepsilon_*$ for the interatomic bond. Comparison of the single vacancy and material with 1% vacancies distribution shows that in the second case the critical deformation is approximately 70% lower. However for the material with defects the critical deformation depends drastically on the occasional mutual location of vacancies, so to obtain more reliable results statistical analysis of a big amount of specimens is required. The results, presented in Fig.6 are measured for the absence of thermal motion. The weak thermal motion ($\Delta \nu = 0.005 \nu_{d}$) decreases the critical deformation for the single vacancy in 3% – 8%. For the specimen with distributed vacancies influence of the mentioned above level of thermal motion was negligible.

Figure 6: Dependence of the critical deformation on the period of loading: 1) single vacancy, vertical lattice; 2) single vacancy, horizontal lattice; 3) 1% vacancies, vertical lattice.

4 Concluding remarks

In the current paper fracture under low-cycle high-amplitude loading of monocrystal material with predefined distribution of defects was studied. Influence of density of vacancies, lattice orientation, loading amplitude, loading period, and interaction characteristics on the fracture process was analyzed. The computations showed that the lattice orientation has great influence on the shape and topology of cracks, growing under cyclic loading. It was shown that the critical deformation is decreasing with the period increase, which is in good correspondence with the numeric and experimental results of material strength dependence on the speed of deformation [10]. The low thermal motion decreases the critical deformation for the single vacancy for about 3% – 8%. The critical deformation for the single crystal material with 1% of vacancies in the considered computer experiment is approximately 70% of the critical deformation of a single vacancy; however this result depends drastically on the occasional mutual location of vacancies.

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References


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