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MODELLING OF CREATION, DEFORMATION AND FRACTURE OF FIBRILLAR MATERIALS

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ABSTRACT

In the present paper the simplest 2D and 3D models of material on the basis of fibrils are proposed. The single fibril is represented as rod consisting of particles which interact via Lennard-Jones potential. In 2D case the creation procedure of the material is proposed. Molecular dynamics simulation of the uniaxial tension of the material is carried out. Stress-strain diagram is obtained. The dependences of the Young modulus on the initial distribution of fibrils and density of the sample are investigated. It is shown that Young modulus grows linearly with the increase of density of the sample. The influence of ordering of fibrils in the sample on elastic properties is investigated. It is obtained that ordering can essentially increase Young modulus in the ordering direction (till 2.5 times). In 3D case simulation of the condensation process of fibrils on the substrate is conducted. Mechanical properties of the obtained material are investigated.

INTRODUCTION

Recently unique mechnical properties of amyloid fibrils were discovered (1, 2, 3). It was shown (1, 2) that they have strength 0.6±0.4 GPa, which is comparable with the strength of steel (0.6-1.8 GPa) and Young modulus 3.3±0.4 GPa, comparable with Young modulus of silk (1-10 GPa). Another important advantage of fibrils is biocompatibility. These facts show that materials on the basis of fibrils can become very promising in the future. In particular, they can find wide application in different areas of medicine (3). In this situation models which can adequately describe processes of elastic deformation and fracture of such material are required. The simplest 2D and 3D molecular dynamics (4, 5) models are proposed in the present paper. Detailed explanation of 2D model can be found in paper (6).

RESULTS

In 2D case the single fibril was represented as two-layer stripe consisting of particles which interact via Lennard-Jones potential. In order to create the material fibrils were randomly added on the plane and connected in the places of the intersections. Computer model of the material is shown in Fig. 1.

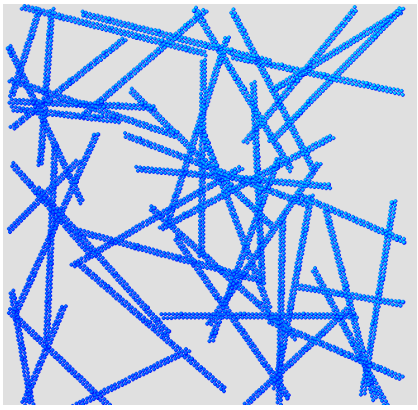

Fig. 1: 2D computer model of the material.

Molecular dynamic simulation of the uniaxial tension was conducted. Stress-strain diagram was obtained. It was shown that fracture occurs at 3% deformation (fracture of the proposed model of the single fibril occurs at 10% deformation). The dependence of Young modulus on the density of the material (number of fibrils per unit area) was obtained (see Fig. 2). One can see that the dependence is linear. The influence of initial distribution of fibrils on Young modulus was investigated. The results of 50 simulations with different initial configurations are shown in Fig. 3. It was obtained that the dispersion of Young modulus caused by randomness of the

initial configuration is approximately 20%. Also the influence of ordering of fibrils in the sample was investigated. It was observed that ordering in one direction can increase Young modulus in this direction till 2.5 times.

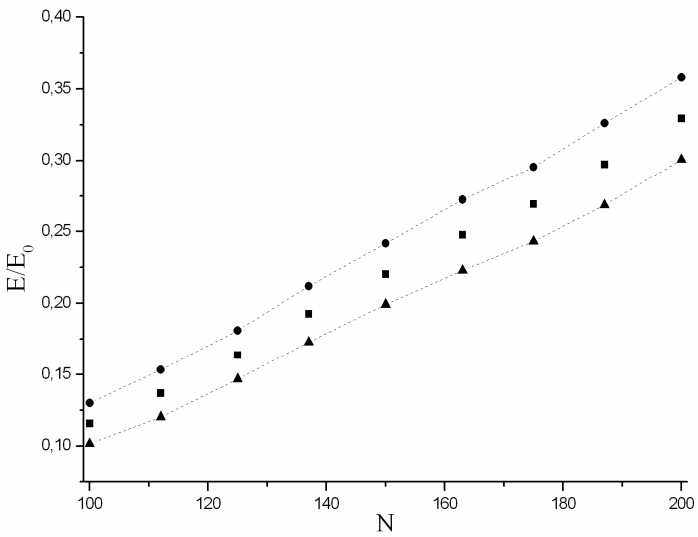

Fig. 2: The dependence of Young modulus E on the number of fibrils. E_0 is Young modulus of infinite monocrystal composed of Lennard-Jones particles. Dotted lines show the dispersion.

Three-dimensional model of the single fibril is shown in Fig. 4. Lennard-Jones interactions between particles which belong to one fibril were assumed. Interactions between different fibrils were described by repulsion part of Lennard-Jones potential except particles which belongs to small areas near both ends of fibrils. These articles were able to attract to each other.

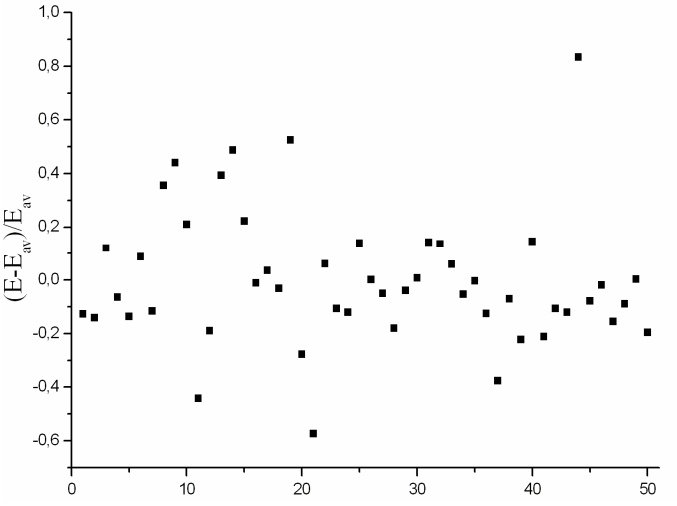

Fig. 3: The dependence of Young modulus E on the initial distribution of fibrils in the sample. E_{av} is average Young modulus.

Initially fibrils were randomly distributed in simulation box. Molecular dynamics simulation of condensation of fibrils on the substrate (bottom of the box) under the action of gravitation was conducted.

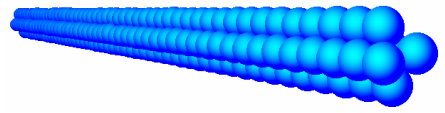

Fig. 4: 3D model of the single fibril.

The sample obtained in the process of condensation is shown in Fig. 5.

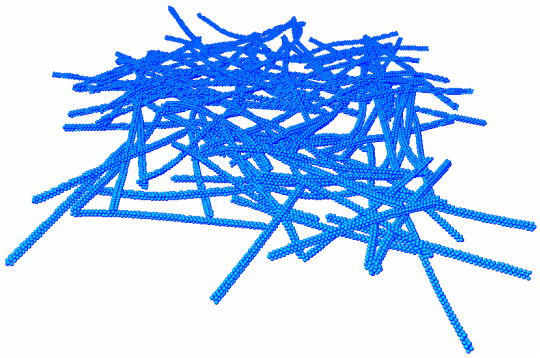

Fig. 5: 3D computer model of the material.

Uniaxial tension test for obtained material was conducted. The stress-strain diagram was obtained. It was shown that fracture occurs at 7% deformation.

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