**Proceedings of the 7th GACM Colloquium on Computational Mechanics
for Young Scientists from Academia and Industry
October 11-13, 2017 in Stuttgart, Germany**

Molecular dynamic study on the tensile deformation of an aluminium nano single- and polycrystal

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Micro Abstract
In our work, we focused on the understanding of the tensile deformation behaviour of a aluminium single- and polycrystal by using molecular dynamics simulations. We considered a fully 3D atomistic model with the embedded-atom method potential for aluminium. A symmetric tilt low energy grain boundary structure was generated and used as an initiation of fracture. Finally, we performed tensile tests investigated the results.

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Introduction

One of the major research topics of the last decade in material science as well as in structural mechanics is the complex field of material failure [7]. The most common used methodologies for the safety assessments of buildings and structures were mainly based on empirical observations, but lightweight construction and extended life time of several constructions require improved material models for more efficient structural design. Typical material failure mechanisms like micro-cracks in quasi-brittle materials, shear bands in metallic materials, grain boundaries or defects and dislocations in the atomic lattice mainly occur on finer scales then the usually applied macro scale. By examining the processes on the finer scales during fracture, valuable insights into the macroscopic material behaviour can be obtained. With molecular dynamic (MD) simulations it is possible to obtain material parameters starting from atomistic tensile simulation and applying homogenization techniques for material parameters on the macro scale [2].

The behaviour of polycrystals is of main interest, since one of the planar defects in polycrystalline materials are grain boundaries (GB) [5]. Polycrystals usually consist of low energy GBs between adjacent crystallites, because materials tend to minimize their potential energy [3]. The GB energy can be critical in the field of stability of grains and the relationship between GB energy and their atomic structure should therefore be investigated to gain a deeper understanding of the properties of the nano structure of materials.

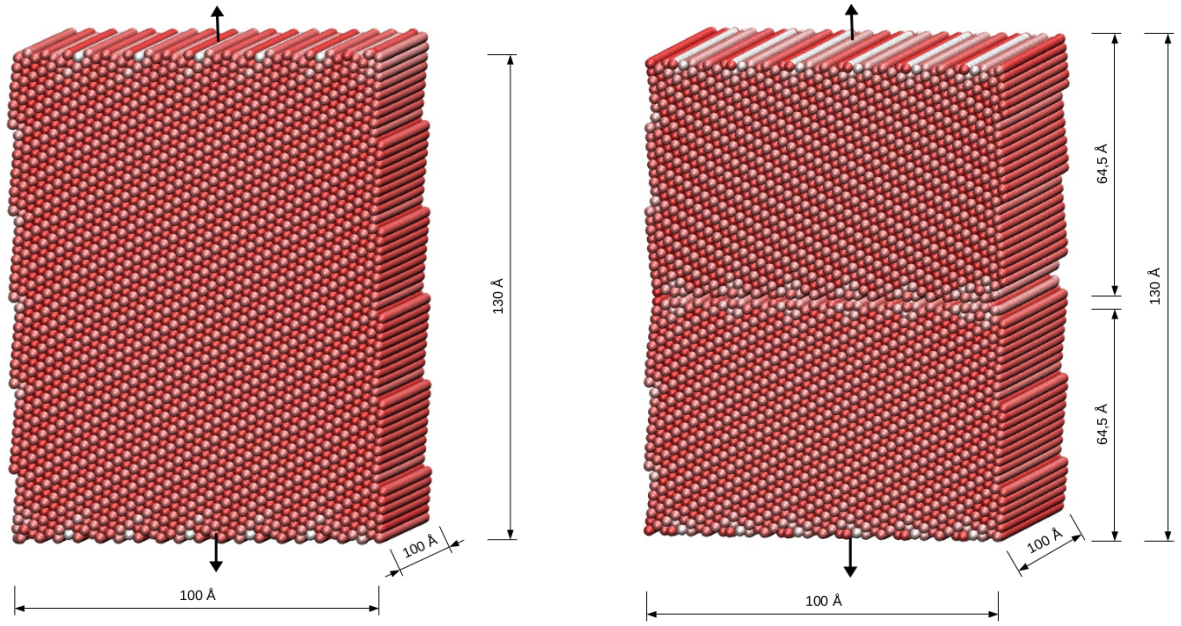
In the last two decades there were many different simulation approaches proposed in the literature to study the micro mechanical tensile deformation of single- and polycrystals at the nanometer scale [1, 3, 5, 6, 8, 9].

The scope of our work is to use MD to simulate and investigate the material and fracture behaviour of a nano aluminium single- and polycrystal in order to have a suitable model for a later embedding in a multi scale model.

1 Methodology

In our investigations, we distinguish between a model of a single crystal and that of a polycrystal, both shown in Figure 1. For each we adopted the 3D atomistic Model from [3], but instead of a

discretization via the quasi continuum method, we considered a fully molecular dynamic model with the embedded-atom method (EAM) potential for aluminum (Al). We used EAM potential



(a) Model of the single crystal without lattice defects

(b) Model of the polycrystal with $\sum 33\langle 111\rangle(2\bar{2}5)$ symmetric tilt grain boundary (STGB) and a gap of 1 Å between the two crystals

Figure 1. Dimensions of the investigated single crystal and polycrystal model

Al99.eam.alloy provided by [4] and adopted it together with a lattice parameter of 4.032 for the FCC lattice. The dimensions of the models are 100Å x 100Å parallel to the interface plane with a heigh of 130Å perpendicular to the interface with approximately 80000 atoms in each simulation box. Before running tensile simulations with the respective model, a minimization of the whole atomic system is accomplished using lattice statics to get a stress free initial state configuration. In case of the polycrystal model this is also necessary to form a bicrystal with a containing grain boundary. The single crystal illustrated in Fig. 1(a) is considered as a perfect crystal without any lattice defects. The polycrystal (Fig.1(b)) in contrast includes a symmetric tilt grain boundary (STGB) of the style $\sum 33\langle 111\rangle(2\bar{2}5)$, which was formed around the middle plane along the y axis by rotating the lattices around the tilt axis. We introduced a small gap of the size 1Å between the two crystals of the polycrystal to have a clear separation before forming a bicrystal later. We applied periodic boundary conditions in all directions. To minimize the system and form a bicrystal with a low energy GB, we used the conjugate gradient algorithm (CGA). As Luther et al. [3] suggested, the energy was calculated within a centered region of 60Å x 40Å x 60Å to exclude some possible disturbances by boundary effects.

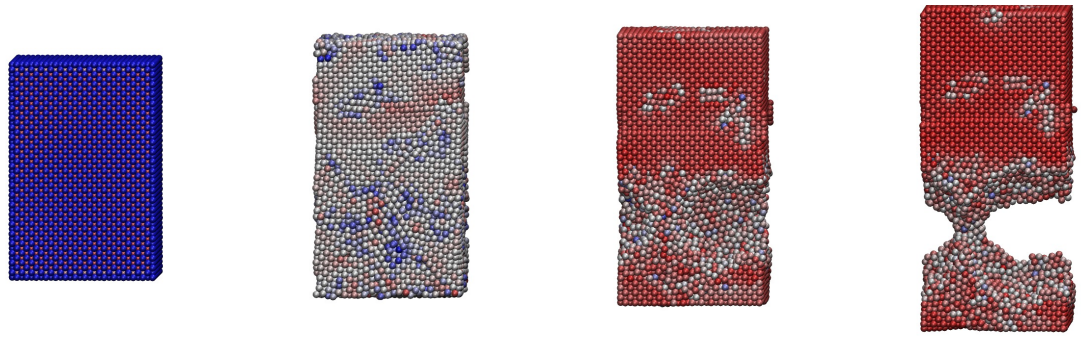
For the geometrical description of the crystal lattice, we used the coincidence-site-lattice description (CSL) scheme proposed by Wolf et al. [8]. The CSL misorientation scheme defines a grain boundary by a relative rotation of the crystallites about the rotation axes n_r through the angle θ and by the normal direction n_1 of the GB [3].

Like Luther et al. [3], the lowest GB energy configuration can be found for a $\sum 33(2\bar{2}5)$ STGB with a misorientation angle of 121.01°.

2 Results and discussion

The simulation procedure was first tested on an Al nano-single crystal before it was applied to the nano-polycrystal containing the lowest GB energy configuration of $\sum 33(2\bar{2}5)$ STGB.

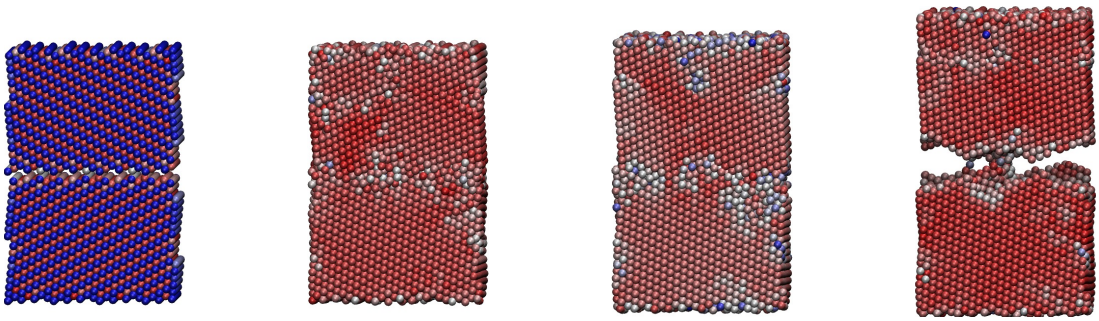
The obtained stress-strain relationship of the single cystal model (fig. 4(a)) shows at the beginning a quasi-linear material behaviour until the maximum stress of 13.0 GPa at a strain of 0.156 is reached. After achieving the maximum tensile strength the stiffness of the material decreases greatly and the material separates. Different snapshots of the simulation of the tensile deformation process are illustrated in figure 2 for the single crystal.



(a) $\epsilon = 0.000$ (b) $\epsilon = 0.099$ (c) $\epsilon = 0.169$ (d) $\epsilon = 0.393$

Figure 2. Snapshots of several simulation states of a nano-single crystal Al.

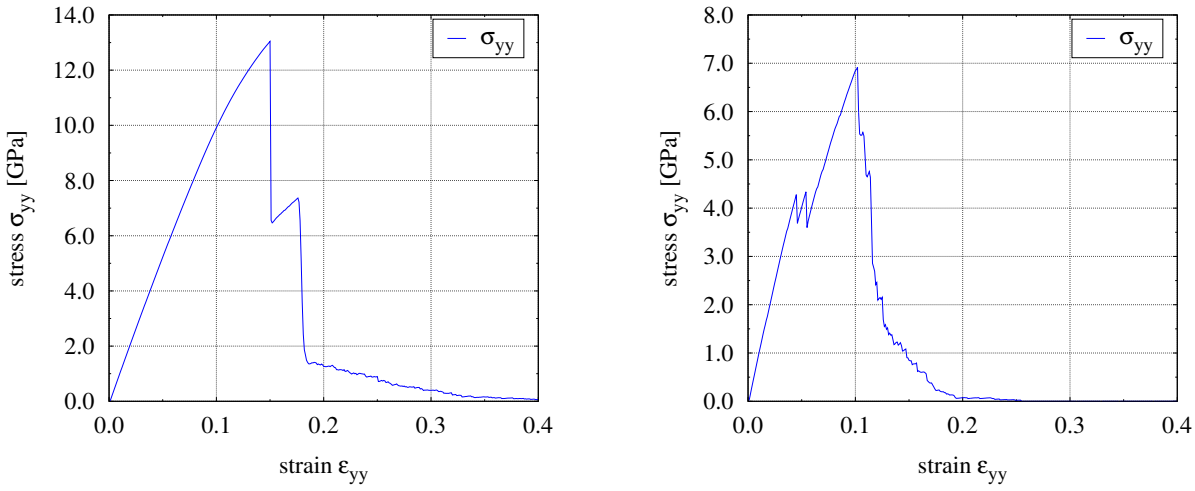
The results of the tensile deformation process of the polycrystal are illustrated in figure 4(b) and are showing a quasi-linear material behaviour until a stress of 4.3 GPa at a strain of 0.045 is reached. That point initiates a pre-damage phase with a small lose of stiffness, but the maximum tensile strength of 6.9 GPa is only reached at a strain of 0.102. Different snapshots of the simulation of the tensile deformation process are illustrated in figure 3 for the poly crystal.



(a) $\epsilon = 0.000$ (b) $\epsilon = 0.045$ (c) $\epsilon = 0.102$ (d) $\epsilon = 0.268$

Figure 3. Snapshots of several simulation states of a nano-poly crystal Al.

Having a view on a macroscopic engineering material parameter like the youngs modulus and comparing it with the values gained out of the nanoscopic tensile tests, shows a big difference. While the experimentally macroscopic tensile test leads to a value of 70.00 GPa for the youngs modulus, the nanoscopic simulation results a much higher value of 101.51 GPa for the single crystal and 102.94 GPa for the polycrystal. This shows that the quasi linear part of the tensile simulation is maybe unaffected by crystal defects. The maximum tensile stress of the single crystal is higher then that of the polycrystal. This can be through the consideration of a grain boundary, as a local dislocation, that decreases the material strength. It is very noticeable that the achieved tensile strength of both models are much higher than those of macroscopic aluminium. The macroscopic material contains a variety of defects like lattice defects, grain boundaries, dislocations, etc., that decreases the overall strength of the material. It could be stated that the material behavior of the nano scale single- and polycrystal is roughly equivalent to that of macroscopic tested aluminium. The material expands, reaches the maximum tensile strength and separates later.



(a) Stress-strain curve single crystal

(b) Stress-strain curve polycrystal

Figure 4. Stress-strain curve single crystal and polycrystal

3 Conclusion

In this study, MD simulation was used to investigate the tensile deformation behaviour of a fully considered atomistic model of a single and a polycrystal for Al. The applied strategy to include a grain boundary as a local defect is well suited, as the material separates along it. The overall material behaviour of the nano-scale models are following the trend of macroscopic tested aluminium, but the obtained values for the maximum tensile strength are too high. Furthermore, an investigation of the influence of material parameters such as the strain rate, the model size and the boundary conditions should be realized.

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