Necking in single-crystal fcc copper nanobeams

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NECKING IN SINGLE-CRYSTAL FCC COPPER NANOBEAMS

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Summary.

Molecular dynamic simulation of nanosized single-crystal copper beams loaded in tension at different strain rates until necking has been performed for two different crystallographic orientations, the [100]- and the [110]-orientations. The molecular dynamics freeware code LAMMPS was employed for the simulations. It was found that, at low enough strain rates, single necking was obtained for both crystallographic orientations and at high enough strain rates both orientations showed necking at both ends. However, the behavior differed between the orientations at intermediate strain rates. For the [100]-orientation multiple necking zones developed which not occurred for the [110]-orientation. This followed from the different developments of the plasticity in the beams between the orientations.

1 INTRODUCTION

Neck formation in tensile beams is known to be a strain rate dependent phenomenon. For low strain rates, usually only one neck is formed. With increasing strain rate, however, multiple necking zones might develop, and one of these can eventually lead to that rupture occurs, so that the beam is split in two. But also after this event stress waves travel through the beam and influence remaining necks and the continued spread of plasticity. This is true at all scales, and here the events at the nanoscale are investigated through 3D molecular dynamics simulations. Single crystal fcc copper beams, with different crystallographic orientations along their length axes, are subjected to tensile loading at different strain rates, and the plasticity spread and the development of necking zones studied. During the loading the evolving disorder in the material is studied through continuously monitoring the losses of symmetries in the initially perfect copper lattice.

2 STATEMENT OF THE PROBLEM

Beams of single crystal fcc copper beams of square cross section size $6a_0 \times 6a_0$ and of length $300a_0$, with $a_0 = 3.615$ Å denoting the lattice constant for copper, were studied. Two different crystallographic orientations were considered. For the first orientation, referred to as the [100]-orientation the coordinate axes (x, y, z), with x along the length-direction, coincide with the crystallographic orientations [100], [010] and [001], respectively. For the second, referred to as the [110]-orientation, (x, y, z) coincide with [110], [-110] and [001], respectively.

Initially the beams were relaxed to equilibrium. Thereafter the load was applied through imposing a constant velocity in the $+x$- and $-x$-directions to atoms within the distance $4a_0$ from each end of the beam, whereas the velocities in the y- and z-directions were put zero for these atoms. This implies clamped ends. No constraints were put on the rest of the atoms.

3 MOLECULAR DYNAMICS SIMULATIONS

The 3D molecular dynamics free-ware LAMMPS, see[1], have been used for the calculations. The interaction between the Cu atoms is described by an EAM-potential developed by[2] and a NVT-ensemble, held at a constant temperature of 0.01K by a Nosé-Hoover thermostat as found in[3,4], is used. The results are evaluated using the Centro-Symmetry Parameter (CSP), cf.[5], as being a measure of the instantaneous lattice disorder. The CSP for an atom is defined according to:

$$CSP = \sum_{i=1}^{N/2} |R_i + R_{i+N/2}|^2 \tag{1}$$

where N is the number of nearest neighbors in the surrounding lattice, equal to 12 for a fcc structure, and R_i and $R_{i+N/2}$ are the vectors corresponding to pairs of opposite nearest-neighbors in the lattice. The value of the CSP signals whether an atom is part of a perfect lattice, in which case $CSP < 3$, or affected by local defects or a geometrical irregularity, in which case $CSP > 3$.

4 RESULTS AND DISCUSSION

Three different loading velocities were applied; $v = v_0/2$, $v = v_0$ and $v = 2v_0$, with $v_0 = a_0/100$/ps, and applied with time step $\triangle t = 5$fs. In Table 1 the strains at initiation of plasticity, ϵ_i, and at rupture through necking of the beams for both orientations and at different applied velocities are seen. For the lowest velocity, $v = v_0/2$, only one rupture, at strain ϵ_{1f}, occurs. For the two higher velocities, two consecutive ruptures through necking occurred, at strains ϵ_{1f} and ϵ_{2f}.

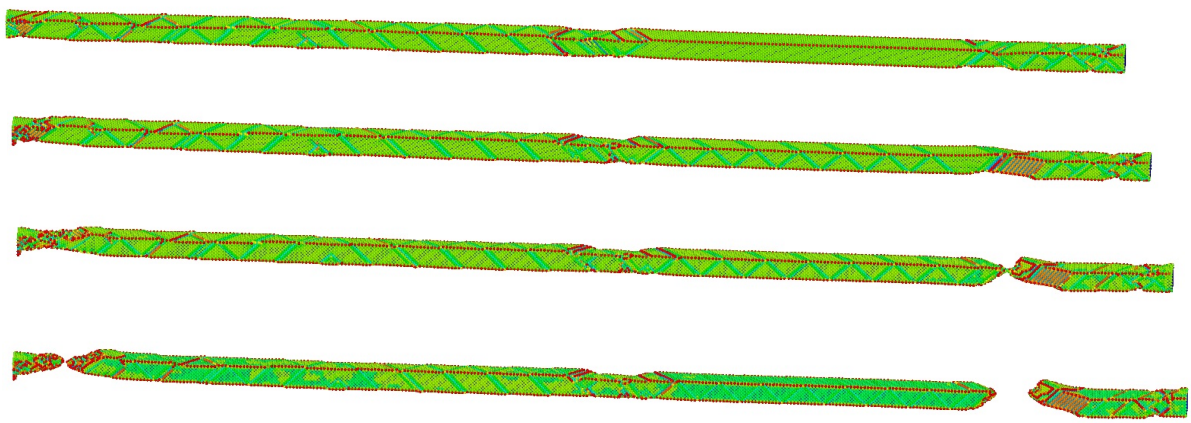

Figure 1: Deformation for the [100]-orientation for $v = v_0$.

For $v = v_0/2$ plasticity spread from the ends of the beams inwards. For the [100]-orientation several limited areas accumulated more plasticity than their surroundings, forming several necking zones. From these, one became dominant and a neck leading to rupture developed. For the [110]-orientation, however, only one necking zone, leading to rupture, was formed.

Figures 1 and 2 show events during deformation for the [100]- and the [110]-orientations for $v = v_0$, respectively. As seen, plasticity due to glide along close-packed {111}-planes spreads along the beams and, at the same time, accumulation of damage occurs in some areas. Several necking regions are formed for the [100]-orientation; for the [110]-orientation necking occurs only in the vicinities of the loaded ends. Eventually one neck leads to rupture for both cases, and the two beam parts are unloaded. However, remaining stress waves cause a second rupture, see Table 1 and Figs 1 and 2. After this second rupture,

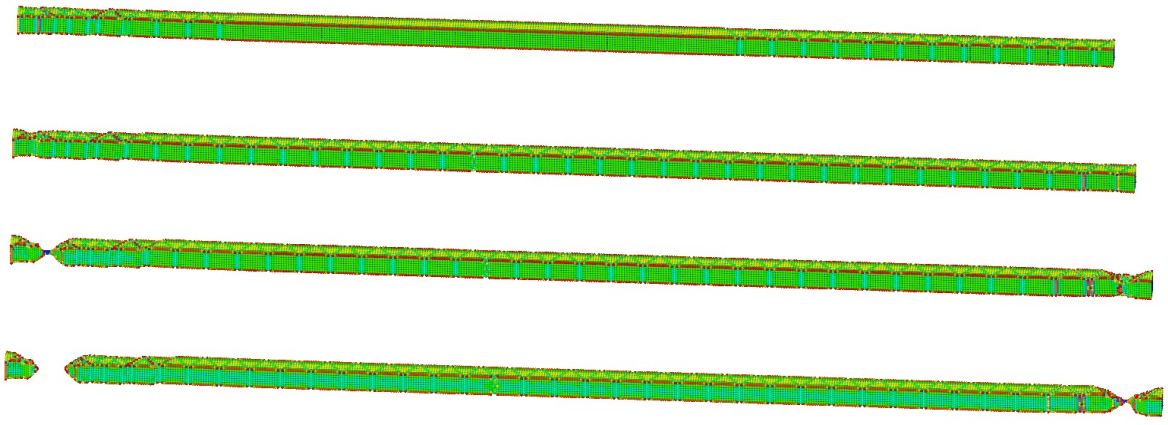

Figure 2: Deformation for the [110]-orientation for $v = v_0$.

	[100]-dir			[110]-dir		
velocity	ϵ_i	ϵ_{1f}	ϵ_{2f}	ϵ_i	ϵ_{1f}	ϵ_{2f}
$v_0/2$	0.187	0.258	-	0.134	0.265	-
v_0	0.0949	0.148	0.166	0.0684	0.130	0.145
$2v_0$	0.0427	0.0650	0.0684	0.0265	0.0573	0.0607

Table 1: Strain at initial plasticity ϵ_i, first ϵ_{1f} and second ϵ_{2f} rupture.

during relaxation, some small amount of plasticity is reversed. The application of velocity $v = 2v_0$ causes almost simultaneous localization of plasticity close to both the clamped ends for both orientations. From these regions plasticity through glide along {111}-planes spreads towards the centres to cover the entire beams and rupture at both ends occur according to Table 1. Further investigations show that increasing the velocity to $v = 3v_0$ gives the same principal behaviour as for $v = 2v_0$, but for this situation the deformations caused by glide along {111}-planes fails to cover the entire lengths of the beams, and the centres of the beams remain elastic.

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