

On the size-dependent mechanical properties of five-fold twinned fcc Fe nanowires

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Summary Fcc bulk Fe is metastable at ambient temperature. However, the existence of five-fold twinned nanowires of fcc Fe at ambient temperature challenges our understandings of the effect of twinned structures. In this study we report the results of a classical molecular dynamics study dedicated to investigate the structural and mechanical properties of the novel five-fold twinned fcc Fe nanowires. Part of the results of the study has been published recently at *Nano Letters*, 11 (2011) 5264–5273 [1]. Some additional results will be presented.

INTRODUCTION

Iron nanorods/nanowires find wide applications in chemical, electrical as well as bio-medical industries. Good understanding of the structural and mechanical properties of the nanowires under thermal and mechanical loading is essential for the design and application of these nanomaterials. It is known that the fcc bulk Fe is thermodynamically unstable at ambient temperature. However, Ling et al have recently discovered that at ambient temperature five-fold twinned nanowire does exist [2]. Classical molecular dynamics simulations have been carried out to explore the role of the five-fold twinned structures on the solid-solid phase transition, elastic properties, plasticity and fracture of fcc Fe nanowires. Fig. 1 shows the atomistic model of the five-fold fcc Fe nanowire analysed [1]. The temperature varied from 0.01 to 1000K and nanowires with four diameter, 6,12,16 and 24nm have been considered. The initial length of all the wires is close to 31.2nm in the ground state.

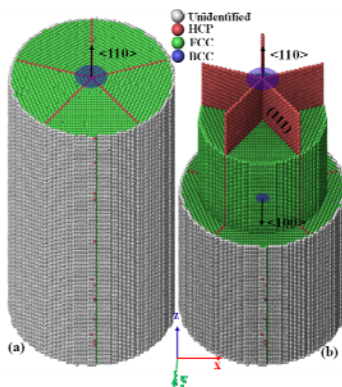


Fig. 1 Atomistic model of the nanowire [1]

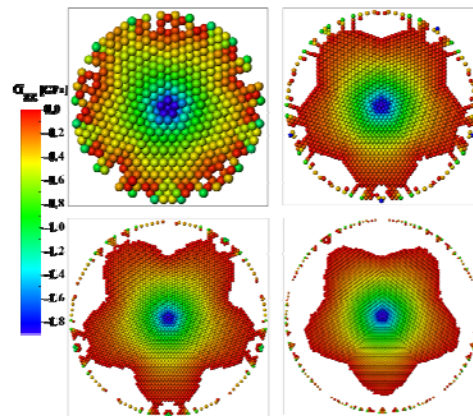


Fig. 2 Intrinsic axial stress distributions of the nanowires At equilibrated states, for the 6,12,16 and 24 nm wires

METHODS

The molecular dynamics code LAMMPS with a Finnis-Sinclair multi-body potential derived by Ackland et al. [3] was used to simulate the five-fold twinned fcc Fe nanowires. The potential has been shown to be able to describe well the structural and mechanical properties of both fcc and bcc phases. In order to avoid the edge effect, nanowires with circular cross section were created. The method and details to generate the unique five-fold nanowire structures were described in [1]. Periodic boundary conditions were applied in the axial (z) direction while the perimeter of the cylinder was free. The nanowire structures were quasi-statically relaxed before any mechanical loading by minimizing the total potential energy using the conjugate gradient method. The Nose-Hoover thermostat was used to keep the temperature constant during the relaxation, while the length was allowed to deform freely based on a Nose-Hoover barostat. Uniaxial straining was achieved after relaxation by homogeneously re-scaling the z-coordinates of all atoms. The Virial theorem has been utilized to estimate the atomic stresses.

RESULTS

Intrinsic stresses and strains at equilibrated state

The five-fold twinned structure plays an important role in the structural and mechanical properties of the fcc Fe nanowires. When the five-fold structure was created, significantly high intrinsic stresses and strains are developed in the nanowires in

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order to accommodate the angular deficiency. Fig. 2 shows the distribution of the monatomic intrinsic axial stress. Unlike the twin-free nanowires where the stress-distribution in the centre is commonly uniform, we observe a star-like stress distribution for the five-fold twinned nanowire. In addition to the outmost layer which has the largest tensile stress large amount of atoms located inside especially along the twin boundaries are also in a tensile state. It is also seen that the tensile stress area fraction increases with the increase of the nanowire diameter. This size-dependent intrinsic stress distribution is an important source of the size-dependent mechanical properties of the five-fold twinned nanowire.

Size-dependent Young's modulus and negative Poisson Ratio

The distribution of the monatomic Young's modulus over the cross section is shown for the smallest nanowire in Fig. 3. Because of the five-fold twinned structures both the monatomic Young's modulus and average nanowire Young's modulus have been found to be strongly size dependent. A local negative Poisson value appears close to the centre of the nanowire (Fig. 4). This finding is the same for all the nanowires.

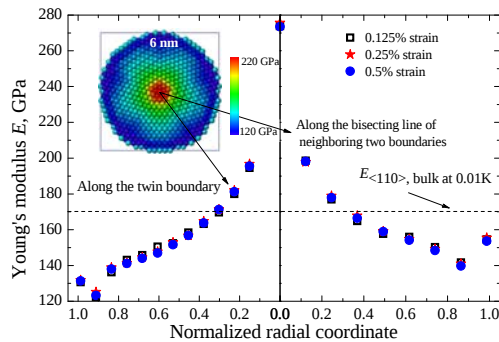


Fig. 3 The monatomic Young's modulus for $n=6$ nm wire

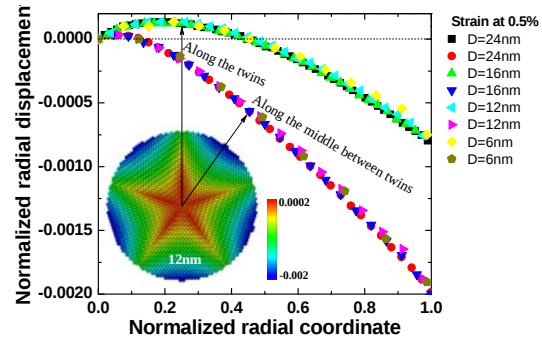


Fig. 4 Normalized radial displacements for the wires

Enhanced solid-solid phase transition and plasticity

A solid-solid phase transition from the initial fcc to bcc structure will occur when a critical strain is reached. The transition starts at the boundary junction and moves into the centre. The phase transition is strongly dependent on the temperature. At low temperature since the thermal atomistic vibration is limited, the critical strain to phase transition is enhanced compared with the middle range temperature (300K). At high temperature the fcc phase turns to be stable, consequently a higher critical strain is expected and plastic yielding by dislocation instead of phase transition will occur first. Thus a U-type critical strain map is obtained for the five-fold twinned nanowires (Fig. 5). The critical strains are also strongly dependent on the wire diameter. When the nanowire increases larger amount of unstable fcc phases contributes to a reduced critical strain.

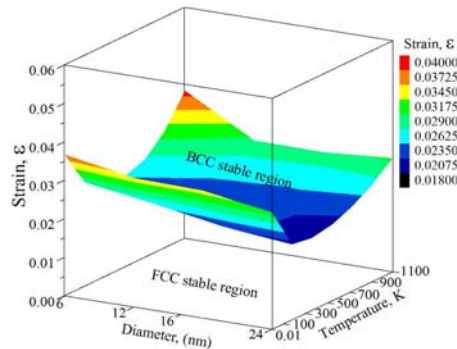


Fig. 5 Temperature and size dependent critical strain plot for the nanowires

CONCLUSIONS

The presence of five-fold twin structure stabilizes the fcc Fe nanowire. The mechanical and structural properties of the five-fold twinned nanowires are strongly temperature and size dependent. A U-type critical strain map is found.

References

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