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Size effect on dislocation nucleation in silicon nanowires

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ABSTRACT

In molecular dynamics simulations of tension, we observed size-dependent brittle-to-ductile transition of the silicon (Si) NWs (Kang 2010). Below *D* = 4 nm, the NWs shows ductile failure behavior associated with dislocation nucleation and glide motion on the primary slip system. In experiments, qualitatively similar trend of ductilefailure behavior was reported (Han 2007) for thin NWs of D < 60 nm.In order to reveal the mechanism behind the size effect of the failure behavior change, the energy barrier for dislocation nucleation is calculated using the freed-end string method. The energy barrier drops almost by half as the diameter reduces from *D* = 7 nm to *D* = 3 nm. This relatively low energy barrier of dislocation nucleation explains the size effect that the thinner the NW is, the more ductile it becomes.

1. INTRODUCTION

Semiconducting nanowires have been fabricated as one of promising nano-structures for the future applications in nano-electro devices. In order for these devices to work reliably and show stable functioning, it is important to study mechanical failure behaviors of the nanowires, because the mechanism behind mechanical failures will give us the ideas relating with how to fabricate the nanowires, how to design the mechanical specs in use, and admissible range of working conditions and more. In our previous molecular dynamics simulations of tensile testing of silicon nanowires with *D* = 3 nm to 7 nm, we have observed the transition of failure behaviors from brittle fracture to ductile one as the nanowire diameter *D* decreases. Silicon is considered as a brittle material when in bulk size and this transition in failure behaviors must be the size effect: the thinner, the more ductile Si nanowires become. In order to explain the size effect in failure behaviors, we investigate the failure mechanisms of Si nanowires under tension.

2. FAILURE MECHANISMS

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In bulk materials, the transition between ductile to brittle failure behaviors is usually explained in terms of mobility change of pre-existing dislocations. The pre-existing dislocations can have different mobility depending on temperature or local stress in non-uniform stress field. For example, Si, a brittle material at room temperature, becomes a ductile material at elevated temperatures due to the increased mobility of dislocations, and this transition is called temperature-induced brittle-to-ductile transition.

However, in the nanowires of a few nanometers in diameter there are no pre-existing dislocations. Even though there are a few, they can be easily sucked out toward the free surfaces due to the image stress. So, when the NW fails, the fracture always starts from the NW free surfaces, the only defected and thus weakest region. From the snapshots of MD simulations, we observed that the ductile failure is associated with dislocation nucleation from the surface. Dislocation nucleation is the very first event in the ductile failure behaviors, which is followed by the sliding fracture, and the nanowire finally breaks into two pieces.

3. THE SIZE EFFECT ON DISLOCATION NUCLEATION

Since the ductile failure is initiated by the dislocationnucleation from the surface, we propose that the dislocation nucleation event is the trigger mechanism to determine failure mode as the nanowire diameter changes. Using the chain-of-states method, we calculated the nucleation energy barrier as a function of the nanowire diameter. As a result, we see that dislocation nucleation energy drops as the nanowire diameter decreases. For example, the energy barrier drops almost by half as the diameter reduces from D = 7 nm to D = 3 nm, which means that dislocation nucleation becomes easier as the nanowire becomes thinner.

4. CONCLUSIONS

To conclude, we observe the failure mechanism of Si nanowires under tension using molecular dynamic simulations, from which the dislocation nucleation triggers the sliding fracture when the thin nanowire fails in a ductile manner. On the other hand, the thick nanowires fail in a brittle manner by cleavage fracture. We calculate the dislocation nucleation energy barrier as a function of NW diameter and the barrier reduces as the NW diameter decreases. This means that for thinner nanowire the dislocations get to nucleate even easier and the NW shows a strong tendency to fail in a ductile manner.

REFERENCES

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