The 2015 World Congress on
Advances in Civil, Environmental, and Materials Research (ACEM15)
Incheon, Korea, August 25-29, 2015

Dislocation Formation Mechanism in Si-Ge Core-shell Nanowires - Molecular Dynamics Study

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ABSTRACT

In the Si-Ge core-shell hetero-structured NWs, the misfit strain, developed at the interface due to the lattice mismatch, is released by formation of interfacial misfit dislocations. Around the misfit dislocation, non-uniform stress of opposite sign develops across the interface. The misfit dislocation can act as a defect source to generate lattice dislocations in the component crystals, which adversely affect the NW performance. In this study, we performed molecular dynamics simulations to investigate the lattice dislocation formation mechanism in [112]-oriented Si-Ge NWs. The formation mechanism is identified by applying slip analysis method at the yield point. We observed that the dislocation of **b**=<110>/2 nucleates at the interface, grows in the shell, and finally swipes through the core region on the {111} plane with highest Schmidt factor as shown in Figure 1.

1. INTRODUCTION

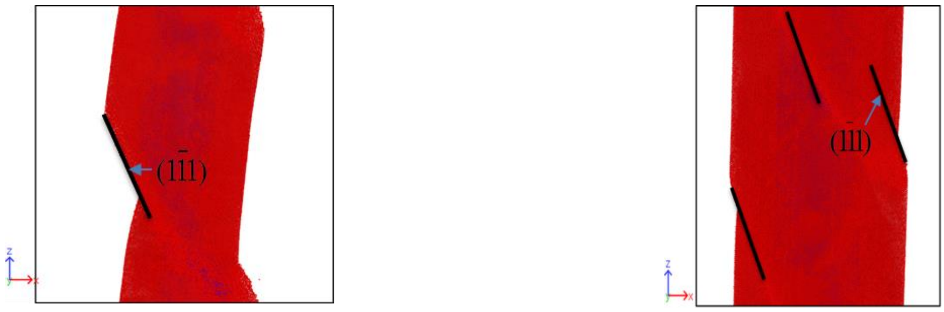
Si-Ge core-shell nanowires have been fabricated as one of promising nano-structures since they show improved electrical properties, such as hole mobility or photoconductivity. In this hetero-structured NWs, there exist misfit dislocations at the interface to relieve the misfit strain that comes from lattice mismatch between core and shell. These misfit dislocations can act as a defect source to generate secondary defects such as lattice dislocations which adversely affect the NW performance. In order to prevent performance degradation, it is important to understand dislocation formation mechanism in the core-shell NWs. We performed molecular dynamics simulations of tensile testing, at 893 K, of NWs with (D, t) = (10, 5) and (15, 7.5) nm, where D is Si core diameter and t is Ge shell thickness. We have observed that the NWs are failed by slip after yielding. In order to acquire full atomistic picture of slip event, we applied slip analysis (Kang 2010) to NW structures.

2. FAILURE MECHANISM

Slip analysis reveals that a secondary dislocation nucleates around the misfit dislocation at the interface between Si core and Ge shell. The lattice dislocation then grows in Ge shell and later expands toward Si core region. The dislocation once sweeps through entire core-shell nanowire on the {111} plane with highest Schmidt factor before failure, regardless of NW diameter. From the simulation, the misfit dislocation indeed acts as a source for the secondary dislocations under mechanical loading.

3. CONCLUSIONS

To conclude, we observe the failure mechanism of Si-Ge core-shell nanowires under tension using molecular dynamic simulations, where the slip event is associated with nucleation of a dislocation of **b**=<110>/2 at the interface and its glide motion on the {111} plane with highest Schmidt factor.



(a) (D,t) = (10, 5) mm (b) (D,t) = (15, 7.5) mm

Fig. 1 Slip in [112]-oriented Si-Ge core-shell NWs. D is Si core diameter and t is Ge shell thickness. In both (a) and (b), the slip event is associated with glide motion of dislocation of **b**=<110>/2 on the {111} plane with highest Schmidt factor

ACKNOWLEDGEMENT
This work was supported by the Yonsei University Future-leading Research Initiative Project of 2015.

REFERENCES

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