The 2013 World Congress on
Advances in Structural Engineering and Mechanics (ASEM13)
Jeju, Korea, September 8-12, 2013

Stability of Eshelby Dislocations in Crystalline Nanowire

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ABSTRACT

The thermally activated escape of Eshelby dislocation in crystalline nanowires is investigated by combining atomistic and continuum models. The energy barrier for dislocation escape from Aluminum <110> nanowires is predicted from an atomistic model as a function of nanowire radius, escape location, and surface step orientation. The dissociation of dislocation into partials has a significant effect on the energy barrier. The dislocation prefers to escape from the nanowire end with extended node, where the dissociaion width is greater than the equilibrium width in the bulk. The energy barrier is further lowered if the surface step aligns with the dislocation's slip plane. A continuum line tension model that accounts for partial dislocation is constructed to reproduce atomistic predictions for aluminum nanowires. The continuum model then makes predictions on the stability of Eshelby dislocations over a wide range of nanowire radii and material types.

1. INTRODUCTION

Due to large surface-to-volume ratio and directional transport properties, nanowires has been attracted research activities as a promising building block for next generation electric device, energy device, and sensors. A key to the realization of nanowire device is fundamental understanding of nucleation and growth process, and controlled growth based on the understanding. One of nanowire growth mode is screw-dislocation-driven (SDD) growth where screw dislocation at the center of nanowire forms a perpetuating surface step at the end of the nanowire, promoting the directional growth. Eshelby is the first to predict that screw dislocation in the nanowire leads to the twisting of nanowire, so-called Eshelby twist. Due to Eshelby twist, screw-dislocations can stay meta-stably, and their stability is related to the feasibility of SDD growth.

Stability of Eshelby dislocation in metal nanowire has been studied by Hirth and Frank [1] where an infinitely long screw dislocation is modeled by line tension model. However, they did not consider the dissociation into two partial dislocations, as well as the nanowire end effect. Thus, in the present work, we employ both atomistic and continuum line tension model to stability of screw dislocation in metal nanowire.

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2. Results and Discussion

Because of large stacking fault energy and relatively small equilibrium distance between two partials, we use aluminum as a model system. Fig. (a) shows the equilibrium configuration of screw dislocation in Al <110> nanowire. Dislocation terminates at a constricted node at the left and an extended node at the right. It can be explain by the partial dislocation's preference to align along their partial Burgers vector near the surface.

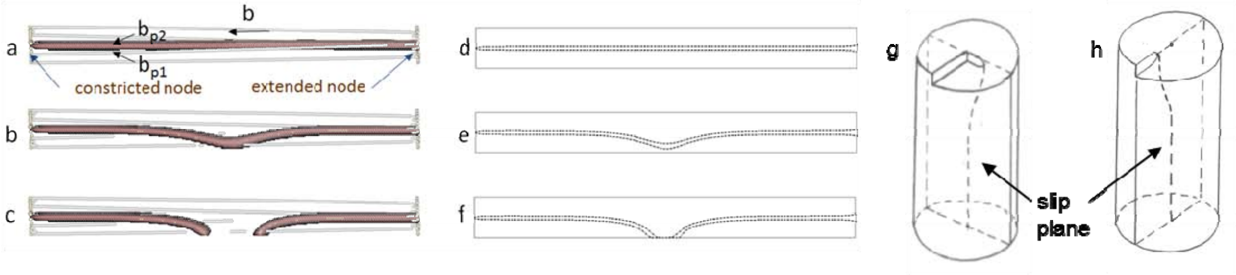

Fig. 1 Atomistic and line tension models of dislocation at metastable state (a,d), activated state (b,e), and escape process (c,f). Diagram for escape from the end, when surface step is nonparallel (g) to the slip plane, and parallel to slip plane (h).

We considered three escape locations for the Eshelby dislocation; from the middle of the NW (M-mode), from the constricted node (C-mode), and from the extended node (E-mode). Fig 1 (b) shows the saddle point obtained by nudged elastic band calculation. We find that as nanowire diameter increases from 4nm to 7nm, energy barrier increases linearly from 1.5 eV to 4 eV for M-mode, from 1.0 eV to 3.5 eV for E-mode, from 1.7 eV to 4.3 eV for C-mode. While both E-mode and C-mode escape create an extra surface step at the end as shown in Fig. 1 (g), their line tension energy costs are about half of that of M-mode, making the total energy barrier results comparable to M-mode. E-mode has less energy barrier than C-mode, since one the partial dislocations is closer to the surface, and attracted stronger by image force from the surface. Next, we considered a special case where the slip plane lies in parallel with the surface step at the end. In this case, as presented in Fig. 1 (h), surface step is removed during the escape of Eshelby dislocation, lowering the energy barrier significantly below that of non-parallel configuration. We find that the energy barrier is lower than 1 eV up to diameter of 15 nm, meaning that Eshelby dislocation is stable if D > 15nm. We develop line tension model reproducing all atomistic results as presented in Fig 1 (d-f) that will be used to model the Eshelby dislocation in various materials.

3. CONCLUSIONS

We study the stability of dislocation in Al nanowire, combining atomistic and continuum line tension model. When statcking fault exist in nonparallel to surface step, Eshelby dislocation can exists if nanowire diameter is larger than 4 nm

REFERENCES

Hirth, J.P. and Frank, F.C. (1958), "On the stability of dislocation in metal whiskers", *Philosophical Magazin,* **3**(34), 1110-1116.