STUDY OF GRIFFITH CRACK NUCLEATION IN A DISCLINATED NANOWIRE WITH A CONTINUUM MODEL

Jun Luo[a)] and Junpeng Zhou
Department of Mechanics, Huazhong University of Science and Technology, Hubei Province, 430074, China

Summary Disclinations and their various configurations are strong sources of internal elastic stress.Relaxation of these internal stresses leads to the formation of other defects, such as cracks, amorphous zones and dislocations. This paper studies the Griffith crack nucleation in a disclinated nanowire with a continuum model. The surface effect of the nanowire is accounted for with the Gurtin-Murdoch model. The Green's functions for the stress fields of a single edge dislocation and a wedge disclination in a nanowire are then solved with the complex variable method. After that, the distributed dislocation technique is adopted to simulate the Griffith crack nucleation. The influences of the surface effect on the material forces applied on the edge dislocation and wedge disclination as well as on the Griffith crack nucleation are then systematically discussed. The current model can be used to predict the critical disclination strength at which a crack starts to nucelate in disclinated nanowire.

INTRODUCTION

A single disclination possesses an energy which is very large in comparison with the energy of a lattice dislocation. Disclinations in solids can only exist in the forms of screened configurations with lower energies, i.e., dipoles, multipoles, loops, or single disclinations screened by free surfaces. An important aspect of these disclination defects is the strong internal stresses associated with them. A variety of relaxation channels of these internal stresses such as crack nucleation, disclination splitting, local amorphization and structure transformation were reported in the literature. Among them, the crack nucleation mechanism has received much attention due to the fact the presence of a crack in solids can drastically decrease their strength.

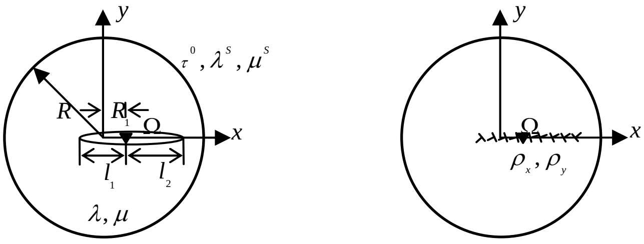
Zhou et al. [1], proposed a continuum model to predict the Griffith type crack nucleations in a disclinated nanowire. They report that in some cases, some discrepancies may be found between the atomistic simulations and continuum predictions. It was concluded that this discrepancy may be due to the surface effect of the nanowire which is often neglected in the continuum model. This paper intends to include the surface effect of the nanowire into the continuum model of the Griffith type crack nucleation in a disclinated nanowire. The surface effect of the nanowire is accounted for with the Gurtin-Murdoch model. The Green's functions for the stress fields of a single edge dislocation and a wedge disclination in a nanowire are then solved with the complex variable method. After that, the distributed dislocation technique is adopted to simulate the Griffith type crack nucleation. The influences of the surface effect on the material forces applied on the edge dislocation and wedge disclination as welll as on the Griffith crack nucleation are systematically discussed.

PROBLEM DESCRIPTION AND SOLUTION SCHEME

The problem to be studied is shown in Fig.1. A nanowire of radius R contains an eccentric wedge disclination with power Ω. The disclination line is parallel to the axis of the nanowire. The nanowire is assumed to be isottopic and its shear modulus and Poisson's ratio are denoted by μ and υ respectively. The surface effect of the nanowire is accounted for with the Gurtin-Murdoch model. The surface tension and surface Lamé constants of the nanowire are given by τ^0, λ^s and μ^s respectively.The eccentric wedge disclination in the nanowire possesses a singular stress field. When the elastic stresses are relaxed, a crack may nucleate. In this paper, we assume that a Griffith-type crack is nucleated in the relaxation process. Thus the crack is opened by the stress fields of the wedge dislincation.

The distributed dislocation technique is adopted to simulate the nucleated Griffith crack. The stress field inside the nanowire is thus the summation of the stress field of the eccentric wedge disclination and that of the distributed edge dislocations with unknown densities. The stress components of the distributed edge dislocations can be obtained through integrations of the stress Green's functions of a unit edge dislocation inside the nanowire along the crack line. The stress Green's functions of a wedge disclination and a unit edge dislocation insid the nanowire are obtained with the complex variable series expansion method. By requiring that the traction free boundary condition should be satisfied at the crack surface. A singular integral equation can be formulated for the unknown densities of the distributed dislocation technique. The singular integral equation can be solved with the numerical method proposed by Gerasoulis [2]. The stress intensity factor of the disclinated crack can be obtained from the dislocation density distributed at the crack tip.

a) Corresponding author. Email: luojun.l@gmail.com.



(a) (b)

Fig. 1 A disclinated Griffith crack in a nanowire and its solution.

RESULTS AND DISCUSSIONS

The influences of the surface effect on the material forces

The stress Green's functions of a single wedge disclination and a unit edge dislocation are solved with the complex varaible method. The material forces applied on a single wedge disclination or a single edge dislocation inside the nanowire can be calculated with the Peach-Koehler formula.

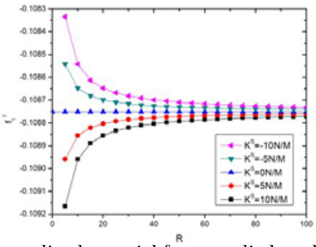


Fig. 2 The normalized material force applied on the wedge disclination.

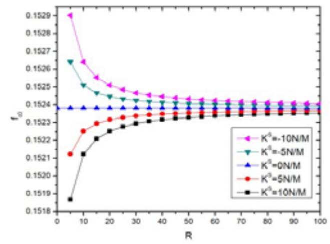


Fig. 3 The normalized material force applied on the edge dislocation.

As we can see from Figs.2-3. The material forces on the wedge disclination and edge dislocation are influenced by the surface effect. However, as the diameter of the nanowire increases, these influences diminish.

The influences of the surface effect on the crack nucleation

We assume that a Griffith crack is nulceated in the nanowire with the elastic stress field of the wedge disclination. The stress intensity factor of the Griffith crack can then be solved with the distributed dislocation technique. We say that the crack can be nucleated when the SIF of the crack exceeds the criticla SIF of the nanowire. The influences of the surface effect on the SIF of the Griffith crack is depicted in Fig. 4.

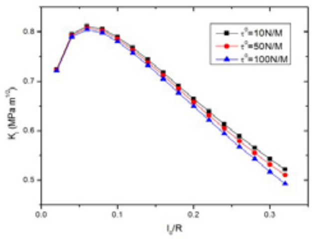


Fig. 4 The influence of the surface effect on the SIF of the disclinated Griffith crack.

We can see from Fig. 4 that the SIF of the Griffith crack is influenced by the surface effect of the nanowire, espeically when the crack tip approaches the surface of the nanowire. This conclusion coincides with that reported by Zhou et al. by atomistic simulations.

CONCLUSIONS

The stress Green's functions of a single wedge disclination and a unit edge dislocation in a nanowire are obtained with Gurtin-Murdoch model and complex variable method. The Griffith type crack nucleation in a nanowire is then studied with the distributed dislocation technique. It is found the that the surface effect has influences on the materials forces of the wedge disclination and edge dislocations. It can also influence the SIF of the nucleated crack.

References

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