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Energy analysis of Zener-Griffith crack nucleation from a disclination dipole

M.S. Wu

School of Mechanical and Aerospace Engineering, Nanyang Technological University, 639798 Singapore

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A B S T R A C T

A disclination dipole can significantly influence the plasticity and fracture of crystalline materials. This paper investigates the nucleation of a Zener-Griffith crack from a disclination dipole under remote loading. The energy formulation leads to a nonlinear algebraic equation, from which the crack length and crack head opening can be determined. The potentiality of the dipole to nucleate a crack is judged by comparing the energy of the uncracked and cracked solid. The results show that both stable submicron-size and unstable micron-size cracks are possible. Not all solutions are energetically favorable. Generally speaking, the unstable crack lengths decrease with the applied stress and the dipole power, while the stable crack lengths increase with these parameters. An opposite trend is predicted for their dependence on the surface energy. In contrast, both stable and unstable crack lengths decrease with the dipole arm length. The crack head opening is generally two to three orders of magnitude smaller than the crack length. The critical dipole power to nucleate a crack increases with a larger surface energy or a smaller elastic stiffness. It has a size effect, in which the logarithm of the critical power decreases linearly with the logarithm of the structural size.

1. Introduction

Disclinations are rotational defects. A wedge disclination is one with Frank vector parallel to its axis. It can be visualized by inserting/removing a wedge of material into/from a cylinder, resulting in a negative/positive disclination. The role of disclinations as rotational defects in the plastic deformation and fracture of crystalline materials is fairly well-established. Romanov and Vladimirov (1992) presented an early comprehensive review of this subject. Subsequently, Romanov and Kolesnikova (2009) reviewed the use of disclinations to describe the structures of grain boundaries, triple junctions, as well as plastic deformation and fracture mechanisms. Recently, Nazarov (2013) also discussed in detail the origin, relaxation and role of disclinations in bulk nano-structured materials.

A disclination by itself possesses a singular stress field both near and far, of the form $\log r$, where r is the radial coordinate. On the other hand, a dislocation stress field varies with $1/r$. One may refer to the classic work of de Wit (1973), or the monograph of Weertman (1996), in addition to the work of Romanov and Vladimirov (1992) mentioned above, for detailed expressions of the stress field. Circular dislocations and disclinations have also been investigated, e.g., Huang and Mura (1970) and Kolesnikova and Romanov (2010). Disclinations often appear in dipole or multipole configurations, with stresses screened at long range. Dipoles have been experimentally analyzed to exist in many metallic polycrystals, including nanocrystals, of aluminum, iron, copper, etc. Klimanek et al. (2001) identified disclinations in various plastically deformed metallic crystals via TEM and other techniques. Murayama et al. (2002) described the observation of disclination dipoles in nanocrystalline iron that has undergone severe plastic deformation via high-resolution transmission electron microscopy. Cordier et al. (2014) resolved disclination dipoles in deformed olivine aggregates

E-mail address: mmswu@ntu.edu.sg.

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by high-resolution electron back-scattering diffraction. They attributed the formation of such dipoles to the lack of slip systems in orthorhombic olivine. Plastic deformation consequently occurs via disclination generation and motion, as evidenced by their experiments.

Research into disclinations and plasticity has received much attention. For instance, Li (1972) used disclinations in the modeling of high-angle grain boundaries. Nazarov et al. (2003) studied the origin and strength of disclinations within triple junctions using the disclination-structural unit model. Gutkin and Ovid'ko (2003) developed disclination models for the generation and development of misorientation bands during the plastic deformation of fine-grained materials. Clayton et al. (2006) investigated the modeling of dislocations and disclinations by micropolar elastoplasticity. Zhou and Wu (2006) derived solutions for a periodic distribution of wedge disclination dipoles in a hexagonal bicrystal. Sundararaghavan and Kumar (2013) used the wedge disclination concept to analyze molecular dynamics simulation results of the compressive yielding of cross-linked epoxies. Taupin et al. (2014) modeled the shear-coupled migration of < 001 > symmetric tilt boundaries which are described in terms of wedge disclination dipoles. Aramfard and Deng (2015) reported a mechanism of dynamic recrystallization via the generation of disclination quadrupoles.

Research of wedge disclination relaxation into other structures or interaction with other defects has also been attempted. Some examples of this research are highlighted in the following. Rybin and Zhukovskii (1978) studied crack nucleation from the triple line of grains and observed that the cracks are often wedge-shaped. Wu and Zhou (1996) investigated the nucleation of a wedge crack from a single disclination in a circular cylinder. Wu (2002) also studied the characteristics of a disclinated Zener crack with cohesive end zones. Zhou et al. (2007) simulated the relaxation of a disclinated nanowire by the atomistic method. Luo and Liu (2011) modeled the interaction of a disclination dipole with a circular inhomogeneity. Fang et al. (2012) investigated the emission of dislocations from disclination quadrupoles. Shodja et al. (2013) studied disclination dipole in an embedded nanowire, taking into account surface/interface elasticity. Xu and Demkowicz (2013) discovered a mechanism for the healing of nanocracks by disclinations.

Despite the advances mentioned above, the problem of crack *nucleation* from a wedge disclination dipole remains to be investigated in detail. Nucleation is of central concern to physicists and metallurgists, since the processing and deformation behavior are influenced by the formation and relaxation of these defects. Experimental work on this problem is quite rare, and theoretical work is limited. The previous work of Wu and Zhou (1996), for example, focuses on the calculation of the stress intensity factors of cracks emanating from a disclination, rather than nucleation of the crack from the defect. Wang et al. (2009) subsequently studied a disclination dipole emanating a Zener crack in the presence of a circular inclusion. It should be emphasized that both works have not really predicted the nucleation event, as the predicted crack length is a result of equilibrium, not of the comparison of energy states. This motivates the current investigation into the fundamental nucleation problem, without other considerations such as elastic anisotropy, inclusions, etc. Furthermore, the previous analytical technique is based on the continuous dislocation modeling of the crack, resulting in rather complicated integral equations. Atomistic methods are highly insightful, but are computationally expensive for parametric studies where it is desired to study the dependences of the solutions on various loading, geometrical and material parameters.

This paper addresses crack nucleation from a wedge disclination dipole, using a composite Zener-Griffith crack model and the energy method. A pure Zener crack is a crack wedged open at one end (the head), resulting in a crack head opening displacement. A pure Griffith crack is one with zero opening at both ends and opens up in response to an applied stress. The combined Zener and Griffith cracks were studied by Weertman (1996), who described in detail the energetics of such a composite crack. The energy method has the advantage of simplicity and requiring moderate computational effort, and allows the determination of both the nucleation event and the length of the nucleated crack (as well as its stability). The disadvantage is that the stress and displacement fields are not determinable via the method, but the advantages are well-suited for the present objective of determining the potentiality of crack nucleation and the equilibrium lengths.

The paper is organized into five sections. Following this introduction, the problem is defined and formulated in Section 2. The computational results are presented in Section 3. A brief discussion follows in Section 4. Conclusions are given in Section 5.

2. Problem definition and formulation

The problem is defined by Fig. 1, which shows a disclinations dipole of strength ω and arm length $2a$ in a linear elastic planar solid. The dipole is two-axis with non-shifted axes of rotation. Other dipoles such as those with shifted axes are explained in Romanov and Vladimirov (1992). Under the stress singularity of the dipole and in the presence of a remote load σ, it is intended to investigate whether the dipole will remain stable or a Zener-Griffith (Z-G) crack will nucleate from it. A Zener crack is characterized by a crack head opening b_T and length $2l$, whereas a Griffith crack by σ and $2l$. If a crack is nucleated, the objective is to calculate both b_T and l. Here, the x-y rectangular coordinate system is attached to the center of the Z-G crack, while the negative and positive disclinations of the dipole are located at $(-l, 0)$ and $(-l-2a, 0)$, respectively. A radius R, interpreted as the structural dimension, characterizes the self-energy of the Zener crack.

2.1. Energy formulation

The energy formulation begins with the development of an expression for the total elastic energy E of the cracked solid. With reference to Fig. 1, the energy of the cracked solid consists of the self energy E_{self} of the disclination dipole and the Z-G crack, the crack surface energy $4\gamma\, l$ (γ is the surface energy per unit area), and the interaction energy E_{int}. The disclination core energy is neglected. Hence: