Stress Intensity Factors for Edge Delamination of Elastic Nano-Films Subject to Chemical Loading

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Abstract

Delamination of elastic thin films from their substrate under thermal or lattice mismatch strain is a classical problem in fracture mechanics. In this paper, we consider this problem where a nanoscale thin film is subject to a combined lattice mismatch strain and a chemical strain induced by solute insertion. The chemical loading differs from its classical counterpart in that the solute-induced strain itself depends on stress distribution in the film, giving rise to a fully-coupled chemo-elasticity problem. In this paper, we adopt a linearized chemo-mechanical model to study the stress intensity factors at the edge of an elastic nano-film on an elastic thick substrate. Within membrane approximation, the problem is reduced to finding solute concentration and stress in a semi-infinite membrane adhered to a substrate. The governing equation is a singular integral equation which is solved semi-analytically. The effect of chemo-mechanical coupling on the stress intensity factors is presented.
Keywords: chemical loading, nano-film, solute insertion, stress intensity factor, delamination.

1. INTRODUCTION

Preserving mechanical as well as chemical stability of the functional materials is a challenging issue in the energy-storage technology. It is well known that thin films of silicon used as anode in lithium-ion batteries lose their stability and integrity during cycling [1]. This loss of integrity is often attributed to the volume changes associated with solute insertion and extraction which is referred to as solute-induced strain. Hence, mechanical failure modes in anodes have been widely studied from both experimental and theoretical standpoints [2-4]. For example, thin films of silicon have been shown to undergo fracture and delamination due to lithium cycling. It has been shown that nanoscale materials, such as nano-films, nano-wires, and nano-particles exhibit a relatively better performance compared to bulk materials [5]. This calls for further theoretical and experimental studies of nanoscale structures and materials under chemical intercalation and deintercalation.

In this paper, we investigate how the coupling between mechanical and chemical fields affects the stress intensity factors at the edge of an elastic nano-film adhered to an elastic thick substrate. The substrate is treated as an elastic half-plane, and the nano-film is treated as an elastic membrane. The interaction between mechanical and chemical fields is taken into consideration utilizing a dilute-concentration limit of the chemical potential.

2. PROBLEM STATEMENT AND FORMULATION

Consider an elastic nano-film of thickness h on an infinitely thick elastic substrate, subject to intercalation induced strain, as well as some initial mismatch strain. The film is considered adhered to the substrate within the region $x > 0$, and delaminated from the substrtate within $x < 0$, as depicted in Figure 1.