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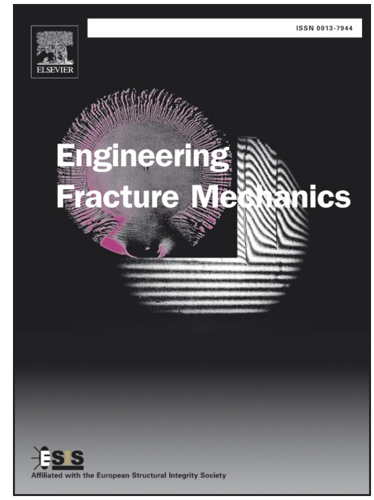

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Dan Johansson, Per Hansson, Solveig Melin

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Stress and displacement configurations in the vicinity of a void in a nanometer copper strip

Dan Johansson[1,a], Per. Hansson[1,b] and Solveig Melin[1,c]

[1]Division of Mechanics, Department of Mechanical Engineering, Lund University, P.O. Box 118, 22100 Lund, Sweden

[a]dan.johansson@mek.lth.se, [b]per.hansson@mek.lth.se, [c]solveig.melin@mek.lth.se

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Abstract. Molecular Dynamics is used to simulate nanometer-sized copper strips. The strips are highly constrained and chosen to mimic thin films between two stiff layers. Further, the strips hold centrally placed straight through crack shaped voids, and are subjected to tensile displacement controlled mode I loading. The tensile stresses and displacements are studied. It is found that if a copper strip is 2.16906nm in a direction orthogonal to the loading direction, the strip does not experience plane strain conditions. However, if this dimension is ≥3.6151nm, the strip shows states of both plane stress and plane strain.

1 Introduction

Technological achievements have over the last decades provided means to design and manufacture nanoelectromechanical systems (NEMS) with high precision. NEMS are employed in a wide range of fields. For example, within medicine NEMS with nanometer thick coatings have been used to detect and sometimes even neutralize specific cells, bacteria and viruses [1-6]. Further, NEMS are used in the manufacture of nanowires, in atomic force microscopy, high density magnetic recording and nanoelectronics [7-11] such as solar cells, modern cell phones and computers. Thus, in everyday life we are surrounded by components that have behaviors and functions that are determined on the atomistic level.

In experiments, materials have on the nanoscale shown behaviors different to those shown on the macroscale. As an example, by using atomic force microscopy Cuenot et al. [12] showed that the elastic modulii of silver and lead nanowires increased as the diameters of the nanowires decreased below 70nm and 100nm, respectively. A similar but more pronounced behavior was observed for polypyrrole nanotubes. In contradiction, [13,14] found that the Young's modulus for chromium nanocantilevers decreased with the size of the cantilever. This behavior was also observed in single-crystalline silicon by Li et al. [15]. These discrepancies evanesce with increasing volume and in an experimentally study of anisotropic single-crystalline copper with specimen dimensions of 30μm×3μm×4μm [16] the measured values of Young's modulus showed good agreements with bulk values. Papers investigating the problem from a theoretical point of view have also been published. It has, for instance, been shown that the definition of how the dimensions of a nanocrystal are measured affects