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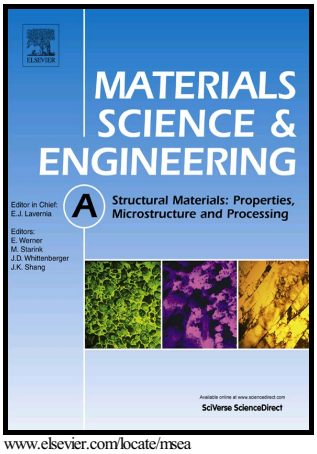

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Effect of crystallographic orientation on nanomechanical modelling of an iron single crystal cracked cantilever beam

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Abstract

Atomistic modelling of 3D, nano-sized, pre-notched cantilever beams of single crystal iron with four different crystallographic orientations has been performed.

The cantilevers proved to be highly affected by crystallographic orientation, displaying very different behavior, ranging from very brittle in the $(100)[0\bar{1}1]$ crack system to very ductile in the $(10\bar{1})[101]$ crack system. The stress intensity calculated using continuum based formulations proved to yield values not correlating well with the observations of brittle and ductile behavior, while the values obtained from a newly developed flange extrapolation method was shown to reflect the qualitative behavior better.

Preliminary examinations in TEM of cantilever beams from machining with FIB has indicated the formation of a local brittle fracture as observed for the brittle $(100)[0\bar{1}1]$ crack orientation in the modelling.

Keywords: Molecular Dynamics, Nanocantilevers, CTOD, Fracture, Iron

1. Introduction

Atomistic modelling has been applied on a pre-notched cantilever of single crystal iron to determine the fracture toughness and reveal the fracture mechanisms at the process zone near the crack tip. The basic motivation for the work is to understand the failure mechanisms in iron and steel, and increase the safety of the application of steel in cold climate.

The main focus has been to investigate the effect of crystallographic orientation and its influence on fracture mechanisms and dislocation activity in the

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