

The Summer Undergraduate Research Fellowship (SURF) Symposium

7 August 2014

Purdue University, West Lafayette, Indiana, USA

Micro-Mechanics Simulation Tool Optimization

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ABSTRACT

Crystalline films grown epitaxially on substrates consisting of a different crystalline material are of considerable interest in optoelectronic devices and the semiconductor industry. One way to progress in this field is to develop simulation tools based on specially designed numerical method. A nanoHUB simulation tool was developed based on the phase field theory, which considers the propagation of dislocations inside the crystalline film. However, the current tool needs several improvements to be more realistic and user-friendly. First, the inputs of the simulation tool are adjusted so that the user can use this tool directly without any additional calculation. The output graphs of this tool are also edited in order to show the dislocation propagation more clearly. Finally, an algorithm was developed to initialize several dislocations in the crystalline film according to the input dislocation density. The new version is much more user-friendly and it considers a more realistic setting with multiple dislocations propagating in the film simultaneously (the current version only considers a single dislocation line). The new tool would serve as a verification of numerical methods and help the understanding of this process.

KEYWORDS

Dislocation, Crystalline Film, Simulation