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A three-dimensional eXtended Element Method for dislocation dynamics

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ABSTRACT

This presentation gives a description of a newly developed dislocation dynamics (DD) method [1]. This method couples an eXtended Finite Element Method (XFEM) for determining the stress fields surrounding systems of dislocations, and level set methods for tracking slip surfaces and dislocation lines. A study of dislocation evolution in strained layer $Si_{1-x}Ge_x$ films will serve to illustrate key advantages of the method, namely the ease of treating anisotropic materials and material interfaces as well as superior scaling properties. An example of such a system is illustrated in Figure 1a along with the computed σ_{xx} stress field for strongly anisotropic material models (Figure 1b).

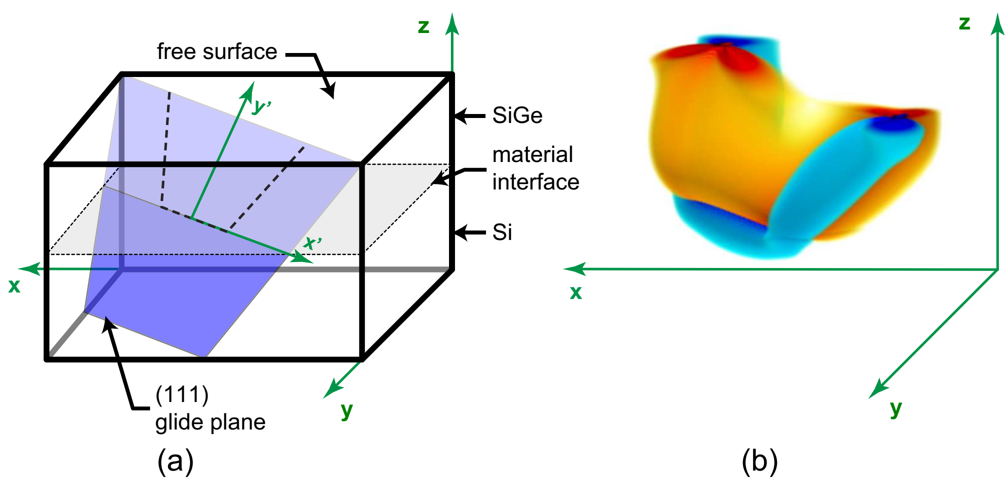

Figure 1: (a) SiGe epilayer on Si substrate with a misfit dislocation segment running parallel to the material interface and connected to the free surface by threading segments. The dimensions of the sample are 2μm×2μm×1μm, where the height of each layer is 500nm. (b) σ_{xx} stress contours near the dislocation core computed with a uniform mesh of 100x100x100 elements (3.1 million degrees of freedom).

The method consists of describing dislocations by two level set surfaces, (f and g), where the surfaces defined by $\mathcal{G} = \{x|f(x) = 0 \text{ and } g(x) < 0\}$ are the slip surfaces and the contours defined by $\mathcal{L} = \{x|f(x) = 0 \text{ and } g(x) = 0\}$ are the dislocation lines. In systems where glide is the dominant mechanism, dislocations can be tracked on multiple two-dimensional planes intersecting a three-dimensional domain. Otherwise, a full three-dimensional level set method is employed.

A discontinuity is added to the standard finite element displacement approximation by a jump enrichment which injects a constant jump equal to the Burger's vector across the glide plane. This is equivalent to the dislocation model first proposed by Volterra [2], where a dislocation can be envisioned by making a cut in a body, introducing a displacement across the cut surfaces and then adhering the two cut surfaces together. Within a specified radius of the core, the displacement approximation is improved by adding a singular enrichment field that is projected onto a coordinate system defined from the gradient of the level set functions and the Burger's vector. For isotropic and weakly anisotropic materials, analytical forms of the enrichment are available. If the material is strongly anisotropic, then the enrichment field can be approximately from a fine-grained, two-dimensional computation.

A key feature of the method is that the enrichment does not increase the degrees of freedom, but rather is constrained by the Burger's vector and the orientation of the dislocations. As a result, the system of equations to be solved does not change as dislocations evolve and the global stiffness matrix need only be assembled on the initial time step. The effect of dislocations therefore only enters as an internal force term that arises from the gradient of the enrichment.

Forces on the dislocation lines are computed either by computing a J-integral or by use of the Peach-Koehler equation. The forces are converted to velocity using a mobility function relating the dislocation force to a velocity through a drag coefficient. The position of the dislocation lines is then updated by projecting the velocity field on the glide plane and advecting the level set field perpendicular to the glide plane.

The computation time of a simulation scales linearly with the number of elements intersected by a dislocation line, allowing much larger systems to be solved than superposition methods which scale by the square of the number of dislocation segments. While previous DD simulation results have been nearly exclusively the product of supercomputing facilities, all results in this presentation were produced on desktop computer.

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