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Combined binary collision and continuum mechanics model applied to focused ion beam milling of a silicon membrane

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ABSTRACT

Many experiments indicate the importance of stress and stress relaxation upon ion implantation. In this paper, a model is proposed that is capable of describing ballistic effects as well as stress relaxation by viscous flow. It combines atomistic binary collision simulation with continuum mechanics. The only parameters that enter the continuum model are the bulk modulus and the radiation-induced viscosity. The shear modulus can also be considered but shows only minor effects. A boundary-fitted grid is proposed that is usable both during the binary collision simulation and for the spatial discretization of the force balance equations. As an application, the milling of a slit into an amorphous silicon membrane with a 30 keV focused Ga beam is studied, which demonstrates the relevance of the new model compared to a more heuristic approach used in previous work.

1. Introduction

Recently, several activities have been targeted on the simulation of nanostructure formation and modification by energetic ion beams, using a "dynamic" binary collision (BC) approach [1–3]. Dynamic BC simulation is a well-established technique for the prediction of compositional changes and sputtering of solids upon ion bombardment [4]. A basic requirement for such a model is the relaxation of the local density changes caused by the implanted ions and relocated atoms. Different solutions have been proposed [1–3] that all share two limitations: First, the directions of material transport during relaxation are chosen in an heuristic manner, whose accuracy is unevaluated. Second, all implementations assume that deviations from the equilibrium densities instantaneously fully relax towards a stress-free state. Therefore, stress is not predicted, which prevents application of the existing approaches to, e.g., the bending of nanowires [5] and membranes [6,7].

Stress relaxation in ion-irradiated amorphous materials is usually assumed to take place via viscous flow. With this material model the bending of silicon wafers due to surface amorphization has been described quantitatively [8]. Radiation-induced viscous flow has also been identified as an important and often the dominant surface smoothening mechanism [9,10], and has been employed in models of spontaneous pattern formation [11,12]. The mechanism of radiation-induced viscous flow has been elucidated by molecular dynamics simulations, supporting a model that identifies point defect generation as the cause of viscous flow [13].

Given the lack of stress representation in existing BC approaches and the well established and reasonably understood model of radiation-induced viscous flow, the benefit of combining the two models is obvious. Such a combined model is the subject of this work. As an application, the milling of a slit into a Si membrane with a focused ion beam is investigated.

2. Model

The new model has been implemented in our binary collision simulator IMSIL. IMSIL has originally been designed for ion implantation in crystalline targets [14], but has been upgraded in recent years for sputtering simulations in one and two spatial dimensions [15,2].[1] In particular, a signed distance function defined as the distance from the surface, with a negative sign outside the target, has been introduced. Stored on a Cartesian grid, it is used to define entrance and exit points of ion trajectories, and to determine the surface normal needed in the planar surface potential model. Another grid (called computational grid here) is used to keep track of compositional changes of the target. To allow extended free flight paths, for

[1] "IMSIL" is now interpreted as an acronym for "IMplantation and Sputtering sImuLator".

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each collision event a set of potential collision partners are determined considering that hit target atoms may also be located in neighboring cells with different composition and density. From these potential collision partners the one with the shortest free flight path is selected. Further details are described in Ref. [2].

As in our previous work [2], the code loops over BC simulation of a certain number of collision cascades and target relaxation. The number of ion impacts in the BC step is chosen as to cause a certain maximum change (e.g., ~10%) in the densities of the cells used to keep track of the spatially dependent target composition. In the relaxation step the nodes of the computational grid are moved, taking with them the material contained in the cells. Finally, a new grid is designed, and the material stored on the relaxed grid is distributed to the cells of the new grid based on the assumption that the material is homogeneously distributed within the relaxed cell.

The proposed model differs from our previous work [2] in two respects. First, a boundary-fitted grid is used to better resolve the surface. In our previous work the surface was defined as the 50% iso-density line of the cell contents, and material outside the surface was ignored in the BC simulation. The error associated with this approximation is relatively minor in the milling of deep trenches (the application studied in Ref. [2]), but turned out to cause severe loss of material in other cases, resulting in sputtering yields that are considerably too high. Second, the target relaxation is now done using a viscoelastic model. These two features are described in the following subsections.

2.1. Computational grid

The computational grid is used both for keeping track of the compositional changes in the BC simulation and for the spatial discretization in the continuum model. Its use in the BC simulation implies that too small cells should be avoided, as otherwise these cells could lose all of their contents during the BC step, which would require special treatment during relaxation. Moreover, for computational efficiency it is desirable that a regular grid be maintained wherever possible, modified only near the surface to resolve it. This is because the determination of the cell index for a given position is a frequent operation in the BC simulation and is much simpler in a regular grid.

Motivated by these two requirements, grid generation is done by starting from a regular grid and adjusting only the near-surface nodes (Fig. 1). For this purpose the intersection points (red dots in Fig. 1) of the surface (thick black solid line) with the midlines (dashed lines) of the regular grid (black solid lines) are determined, which yields segments describing the surface (red lines). Each segment belongs to one cell of the midline grid, the center of which is a node of the regular grid. This node is moved to the center of the (red) surface segment. In this way excessively small or large cells are avoided provided the surface is sufficiently smooth. Concave quadrilaterals may occur in concave sections of the surface. They were not found to cause problems in the BC simulation or during relaxation, however.

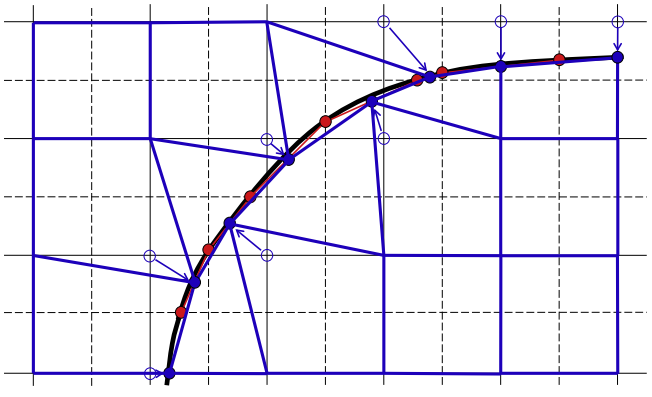

Fig. 1. Construction of the boundary-fitted grid from a regular grid. Thick black line: surface; thin black lines: regular grid; black dashed lines: midline grid; red dots: intersection of the surface with the midline grid; blue dots: nodes moved from regular grid positions to the surface; blue lines: final grid. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

2.2. Viscoelastic model

The feature that distinguishes ion bombardment from most other sources of stress is the distributed loss or gain of material. Stress relaxation takes place simultaneously to this local change in mass (if times within collision cascades are not resolved). To avoid the computational effort resulting from an excessive number of relaxation steps, a certain number of ion impacts has to be simulated in a BC step with the target geometry fixed to that at the beginning of the step. Consequently, the BC step yields the atomic densities N that would be observed if no relaxation took place. Assuming isotropy and purely elastic dilatation, pressure can be related to this density by

$$p = K\left(1 - \frac{N^*}{N}(1+\varepsilon_V)\right), \tag{1}$$

where K denotes the bulk modulus, N^* the equilibrium density, and ε_V the volume strain. Strain is defined here with respect to the situation at the beginning of the relaxation step [16] rather than with respect to a stress-free state.

The constitutive relation of a viscoelastic material ("Maxwell body") is given by

$$\frac{1}{G}\frac{\partial \boldsymbol{\sigma}'}{\partial t} + \frac{1}{\eta}\boldsymbol{\sigma}' = 2\frac{\partial \boldsymbol{\varepsilon}'}{\partial t}, \tag{2}$$

where G denotes the shear modulus, η the viscosity, t time, and $\boldsymbol{\sigma}'$ and $\boldsymbol{\varepsilon}'$ the deviatoric parts of the stress and strain tensors, respectively [16]. This equation is discretized with respect to time using the Backward Euler method. Using the symbols $\boldsymbol{\sigma}'$ and $\boldsymbol{\varepsilon}'$ for representing values at the end of the time step Δt and $\boldsymbol{\sigma}'_0$ and $\boldsymbol{\varepsilon}'_0$ for values at the beginning of the time step we obtain

$$\boldsymbol{\sigma}' = \frac{g}{G}\boldsymbol{\sigma}'_0 + 2g\boldsymbol{\varepsilon}' \tag{3}$$

with

$$\frac{1}{g} = \frac{1}{G} + \frac{\Delta t}{\eta}, \tag{4}$$

We have used $\boldsymbol{\varepsilon}'_0 = 0$, since it turned out sufficient for the present study to use one time step per relaxation step. $\boldsymbol{\sigma}'_0$ is equal to $\boldsymbol{\sigma}'$ of the previous relaxation step.

Eqs. (2) and (4) have been written in terms of a regular viscosity η (units [Pa·s]). Assuming that radiation induced viscous flow is driven by atomic displacements [13], the radiation-induced viscosity η' may be defined by

$$\frac{\Delta t}{\eta} = \frac{n_{\mathrm{dpa}}}{\eta'} \tag{5}$$

with n_{dpa} the number of displacements per target atom during time step Δt, and η' in units of [Pa·dpa]. n_{dpa} is calculated from the deposited nuclear energy using the modified Kinchin–Pease model [17].

The displacements of the grid nodes are obtained by writing the strain tensor in terms of the displacement vector components in the usual way and solving force balance equations for volumes surrounding each node. The displacement vector components are