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Quantifying eigenstrain distributions induced by focused ion beam damage in silicon

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ABSTRACT

Eigenstrain offers a versatile generic framework for the description of inelastic deformation that acts as the source of residual stresses. Focused ion beam (FIB) milling used for nanoscale machining is accompanied by target material modification by ion beam damage having residual stress consequences that can be described in terms of eigenstrain. Due to the lack of direct means of experimental determination of residual stress or eigenstrain at the nanoscale we adopt a hybrid approach that consists of eigenstrain abstraction from molecular dynamics simulation, its application within a finite element simulation of a flexible silicon cantilever, and satisfactory comparison of the prediction with experimental observation. Directions for further enquiry are briefly discussed.

Keywords:

Focused ion beam milling
Molecular dynamics
Eigenstrain
Residual stress

The concept of eigenstrain was introduced by Toshio Mura [1] as a means of describing various kinds of inelastic deformation that serves as the source of residual stresses. Over the last three decades, developments in eigenstrain theory have shown the flexibility and versatility of this approach [2], as well as its suitability for different scales of consideration, from macro- to meso- to micro-scale [3]. The present study deals with the adaptation of the output from atomistic scale modelling and experimentation to the description of the consequences of Ga⁺ ion beam milling accompanied by ion implantation and damage [4].

In the context of nanoscale analysis of strains and stresses, linking atomistic data to equivalent continuum descriptors presents a considerable challenge, since in this context the very classical concepts of strain and stress come into question. Whilst strains are conventionally defined in terms of dimensional and shape changes with respect to a reference configuration, frequently at nanoscale the reference state is not specified, nor possible to define it due to the indistinguishability between identical atoms. A particular challenge arises when the original configuration is not a perfect crystal, but rather an amorphous or highly defected structure.

Extraction of stress values from molecular dynamics (MD)

result is based on the Virial Theorem [5]. The state-of-the-art is described in a recent review [6].

In the present study we address the issue of strain and stress due to focused ion beam damage on target material. The motivation comes from the increasing use of FIB milling for TEM sample preparation (lamellae), various flavours of micro-scale sample machining, e.g. for micro-cantilever bending, toughness testing, micro-pillar fabrication for compression testing and splitting [7,8]. Ion beam modification of the near-surface layer of material causes changes in the mechanical state that need to be taken into account to draw correct conclusions. Residual stress consequences of ion beam milling have been brought into sharp focus by the recent advances in FIB-DIC micro-ring-core milling for residual stress evaluation [9,10]. This approach has become more firmly established in the past decade as a highly versatile and widely available method finding applications in micro- and nano-scale structural design. The most frequently used experimental configuration employs a combination of FIB and SEM for material removal and imaging, respectively. FIB milling operates by transferring the momentum of energetic ions (often Ga⁺, but also heavier ions such as Xe in plasma FIB systems) to the atoms of the target material. This process causes not only the ejection of secondary ions, but also results in the primary ion implantation within the target, accompanied by a damage cascade that causes structural modification (proliferation of defects such as stacking faults, creation of

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Frenkel pairs of interstitial atoms and vacancies, dislocations, voids). The totality of the associated permanent inelastic deformation corresponds to *eigenstrain*.

The induced ion beam damage can be classified into different levels of severity as a function of interaction conditions and structural modification induced. For example, in [11] the first level corresponding to low ion fluence (number density of ions impinging on a unit surface area) yields a shallow implantation region of small isolated defects, and a linear relationship between defect volume fraction and the induced inelastic strain (eigenstrain). The second level of ion damage is characterised by accelerating loss of atomic regularity (crystallinity), accompanied by increases in defects size and density, leading to semi-crystalline state. At the third level significant disruption of crystal lattice leads to amorphisation and is typically associated with material swelling and expansive eigenstrain.

The passage of an ion through target material can be simulated using SRIM code [12] that allows the determination of stopping distances and the resulting distribution of incident primary ions and damage within the material. However, since in the present study the primary interest is in the overall stress-strain state within the target, more detailed simulation needs to be conducted within the modelling framework of Molecular Dynamics (MD) that has been used extensively to study the atomic structure evolution with temperature and mechanical deformation for a vast range of materials [13].

In the present study the effect of Ga⁺ ion beam milling on the damage and residual stress state in single crystal silicon substrate was evaluated using LAMMPS molecular dynamics code [14].

The model setup illustrated in Fig. 1 involved a material volume containing up to ~500,000 silicon atoms with the dimensions of $22 \times 8 \times 22 \text{ nm}^3$ and $20 \times 7 \times 69 \text{ nm}^3$ for the ion energies of 5 keV and 30 keV, respectively. (001) and (111) surfaces were irradiated by up to 400 Ga⁺ ions at the grazing angle of 10° from the surface plane. In-plane periodic boundary conditions were imposed. Si-Si interactions were described by the modified semi-empirical Stillinger-Weber potential [16] merged with the Ziegler-Biersack-Littmark (ZBL) potential [12] for short interatomic distances. Ga-Si interactions were described by the ZBL potential. Collision cascade simulations were performed within the NVE thermodynamic

ensemble using a variable time step for a maximum of 15 ps. A thermostat wall at 300 K was used to dissipate the incident ion kinetic energy [15]. Atoms leaving the simulation box were removed from the system (considered sputtered). Atomic stress tensor was obtained by averaging of Virial stress over 10 ps, with Voronoi volume evaluated for each atom (see [14] for further detail). Residual stress depth profiles illustrated in Fig. 2(a) and (b) for 10° grazing angle incident Ga⁺ ion beams of energy of 5 keV and 30 keV, respectively, show variation from superficial tension to sub-surface compression. Incident ion beam energy affects both the depth of modification and the magnitude of induced residual stress.

Eigenstrain as a means of bridging the scales relies on abstracting inelastic permanent strain from finer scale and applying it as a perturbation at the coarser scale. The task of determining the underlying eigenstrain from residual stress information (e.g. from MD) represents an inverse problem [2]. The material volume dimensions and boundary conditions were replicated in a Finite Element model. The variation of elastic properties from pristine crystalline Si to those of the amorphized layer were described by a smooth function, with Young's moduli values taken from the literature [17,18] to be $E_{\text{cryst},111}=188 \text{ GPa}$ and $E_{\text{amorph.}}=80 \text{ GPa}$, respectively.

The present study aims to validate several conceptual connections, notably between MD results and the abstraction of eigenstrain profile, and between the eigenstrain-based FE simulation of the deformation of a particular flexible member (AFM cantilever) and the observation of its curvature after ion beam milling in FIB-SEM [4]. Consequently, the previously described geometry of a thin flexible silicon cantilever free from pre-existing residual stress subjected to 30 keV Ga⁺ ion milling at normal incidence [4] was adopted. Since experimental FIB milling was conducted at normal incidence, MD simulations we also performed for this beam-sample interaction geometry, with other conditions similar to those described above. The results of the eigenstrain-based FE simulation illustrated in Fig. 3(b) illustrate that the elastic strain profile calculated from the FEM compares satisfactorily with the outcome of MD simulation, as shown in Fig. 3(a).

The radius of curvature of the cantilever predicted by the FE simulation using the eigenstrain profile abstracted from MD

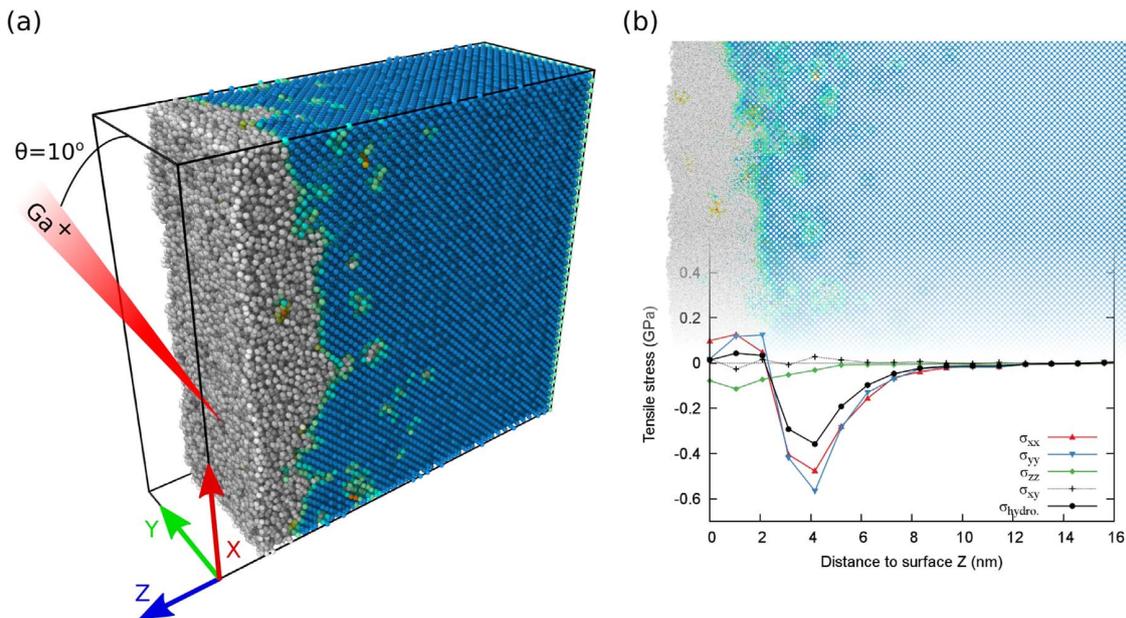


Fig. 1. The illustration of (a) MD model setup, simulation geometry and (b) output.

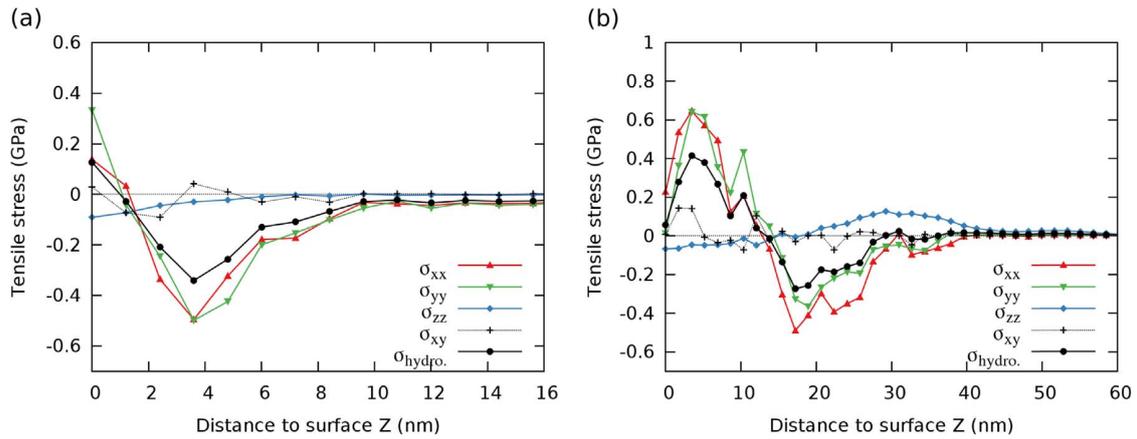


Fig. 2. Residual stress profiles as a function of depth below the surface for the ion energy for (a) 5 keV and (b) 30 keV, respectively [14].

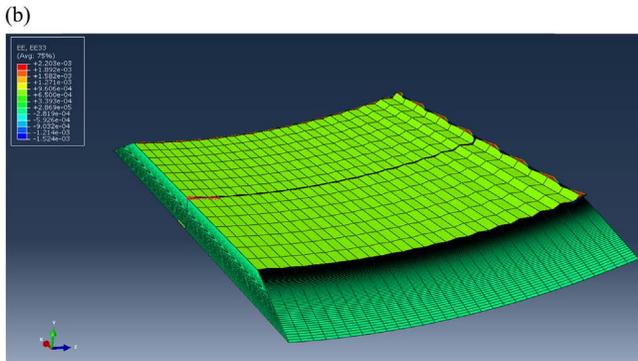
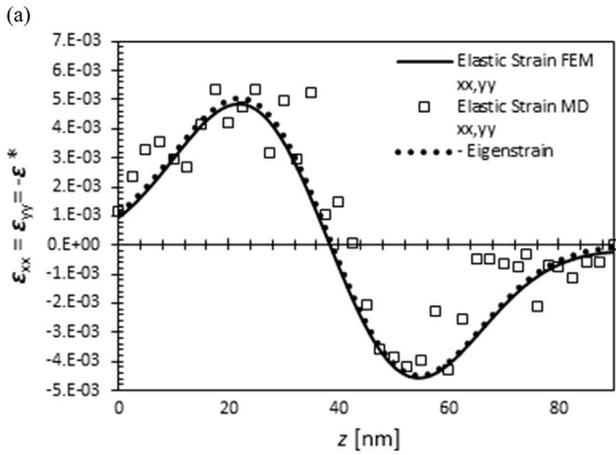


Fig. 3. (a) Abstraction of strain and eigenstrain from the residual stress results of MD simulation. (b) The result of the incorporation of eigenstrain in the continuum FEM simulation.

simulation is 36.8 mm. In comparison, the experimentally observed curvature radius reported in [4] was 40.8 mm. The difference of $\sim 10\%$ between these results is likely to be associated with the fine details of ion flux on the sample, but the disagreement may be reduced further by careful calibration.

The approach described in the present study provides a basis for further parametric evaluation of focused ion beam damage eigenstrain effect as a function of fluence, incidence angle, and energy.

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