

Finite element modeling of nanoindentation and scratching of Si, SiC, Ge crystals with anisotropic plasticity

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Abstract. Parameters of Hill's anisotropic elastoplasticity for diamond and Si, SiC, Ge semiconductors have been estimated from nonlinear stress-strain curves obtained by computational quantum chemistry. Using these parameters, finite element modeling of nanoindentation with Berkovich pyramid and frictionless scratching with spherical tip have been carried out. It has been shown, that the plastic anisotropy leads to the hardness anisotropy commonly observed by experimental indentation of (111), (011) and (001) crystallographic surfaces of the diamond-like crystals. The creep flow has been regarded in a quasi-static approach. Propagation of a median crack has been accounted by cohesive zone model.

1. Introduction

Indentation [1] is a common method of experimental determination of hardness and elastic properties of materials. In particular, nanoindentation and scratching experiments are widely used for testing thin film heterostructures. Since the indentation theory lacks analytical solutions, it is accompanied by computer modeling by finite element method (FEM), which requires data on plastic behavior of a material from other experiments, such as axial deformation of a rod beyond elastic linearity limit. However, a lack of such experimental data for materials of interest in turn forces researchers to calculate necessary properties of the materials by means of computational chemistry, especially when it comes to single crystals possessing all kinds of anisotropy. Indeed, for orthotropic materials (such as cubic diamond-like crystals C, SiC, Si, Ge), when compared to isotropic ones, not only the elastic anisotropy arises, when the shear modulus G becomes independent from the Young's modulus E and the Poisson's ratio ν , but the plastic anisotropy arises as well, when the elastic limit (yield point) for shear stress σ_Y^s becomes independent from the one for axial stress, e.g. compressive yield stress σ_Y^c , as we are going to consider an indentation process that generally comprises only shear and compressive strains. The independent pair of shear and compression elastic limits can be described by Hill's parameter h of plastic anisotropy [2]:

$$h^{s/c} = |\sqrt{3} \sigma_Y^s / \sigma_Y^c|. \quad (1)$$

If $h = 1$, the equation becomes the Mises' criterion of isotropic plasticity.

2. Parameters of anisotropic elastoplasticity

In our previous work [3], the nonlinear stress-strain curves up to creep or fracture limit for shear and axial deformations of C, SiC, Si, Ge crystal cells were calculated by computational quantum chemistry in ABINIT software for the ground state at $T = 0$ K by two methods: DFT LDA with TM



pseudopotentials and DFT GGA with ONCV pseudopotentials. The averaged result for the current application is presented in the table 1. Limits of linear elasticity were estimated by bilinear approximations of the curves with logarithmic Hencky strain, so the resulting elastic constants don't necessarily coincide with the usual values for small strains near the equilibrium. The nonlinear parts of the curves represented only anharmonicity and didn't represent plastic irreversible deformations, since there were no corresponding crystal defects that appear at bigger scales and temperatures. So, the actual plastic yield points may differ from the linear limits obtained in this way, however there should be a correlation between them, which leads to the same Hill's relation, not to mention that computed fracture limits usually coincide with the experimental data, so moving only the yield point doesn't affect the bilinear curve very much. For FEM calculation beyond the ultimate strength, where creep or fracture occurs, we use a low-angle line of stress-strain dependency (1 or 5 % of the plastic line slope) to remain in equilibrium quasi-static approach (figure 1).

Table 1. Input data for FEM computation with multilinear hardening law exemplified by figure 1. Yield (γ) and ultimate (U) stresses σ for compression (c) along [001] crystallographic axis and for shear (s), accompanied by the corresponding axial ε and shear γ strains. Poisson coefficient ν actually depends on strain, a value at zero strain is used for stiff diamond C, while a representative value at compressive yield point is taken for other materials. $h^{s/c}$ is the Hill's anisotropic plasticity ratio between shear and compression, which is generally different from the one for tensile deformation [3].

| | ε_Y^c | ε_U^c | γ_Y | γ_U | σ_Y^c (GPa) | σ_U^c (GPa) | σ_Y^s (GPa) | σ_U^s (GPa) | ν | $h^{s/c}$ |
|-----|-------------------|-------------------|------------|------------|--------------------|--------------------|--------------------|--------------------|-------|-----------|
| Ge | -0.045 | -0.15 | 0.055 | 0.21 | -4.4 | -9.5 | 3.7 | 12.1 | 0.307 | 1.46 |
| Si | -0.065 | -0.18 | 0.094 | 0.24 | -7.3 | -12.3 | 7.2 | 15.5 | 0.304 | 1.71 |
| SiC | -0.107 | -0.30 | 0.175 | 0.32 | -27.9 | -49.8 | 42.7 | 64.8 | 0.297 | 2.65 |
| C | -0.161 | -0.27 | 0.216 | 0.34 | -161.8 | -219.8 | 117.6 | 141.5 | 0.114 | 1.26 |

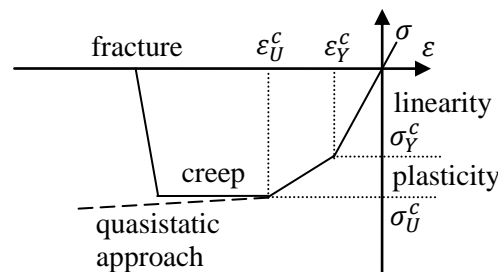


Figure 1. Schematic stress-strain curve by the example of compression. The quasistatic approach to the creep line is used in the FEM calculation beyond ε_U^c .

3. Indentation with Berkovich tip

Diamond three-sided Berkovich pyramid has its sides inclined at 65.27° angle to its geometrical axis aligned to the [001] crystallographic axis. The pyramid has been modelled with 100 nm tip curvature common for standard nanoindenters. FEM calculation of the 150 nm indentation process with account of Hill's anisotropic plasticity has been carried out in ANSYS software. Normal Lagrange formulation for frictionless contact between the bodies has been chosen to exclude penetration error, which has crucial importance in this kind of simulation. Combined symmetry of the indenter and the crystal sample has been taken into account to reduce the computational problem. Different rotational orientations of the pyramid in respect to the crystal surface may physically lead to a bit different results, but this difference happened to be within numerical error.

Figure 2 shows an example of the FEM model with residual plastic strain after indentation. Most of the plastic strain is accumulated under the pyramid edges, where cracks are usually observed in the experiments. Formation of a main median crack has been calculated by cohesive zone model (CZM), using data on the fracture stress limits from the table 1 and data on the crack surface energy ($\sim 2 \text{ J/m}^2$ for Si) calculated by computational quantum chemistry in [4]. The formation of crack hasn't impacted the value of the reaction force.

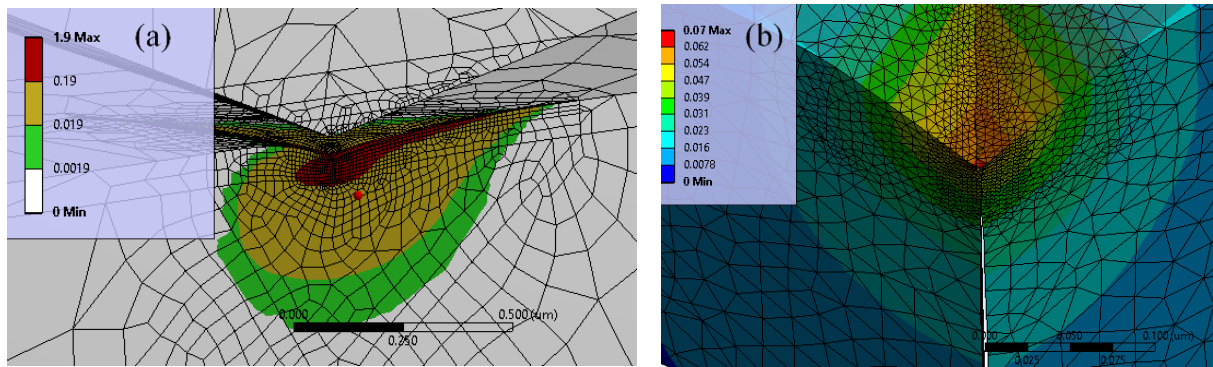


Figure 2. Section view of the finite element models of indentation of Si(111) surface: (a) after 150 nm indentation with residual equivalent plastic strain plotted in logarithmic colormap, (b) median crack (white color) propagation by cohesive zone model at 70 nm indentation with total deformation plotted in color. Vertical projection of the pyramid edge is aligned to the Si $[2\bar{1}1]$ axis.

Figure 3 clearly shows by the example of silicon that the presence of plastic anisotropy leads to the different reaction forces for different orientation of the crystal sample, as it is commonly observed in the experiments. The Hill's parameter $h > 1$ reduces amount of plastic strain, thus narrowing the loading-unloading curves. Calculated hardness is 12.1 GPa, 11.8 GPa, and 10.9 GPa for Si(111), Si(011), and Si(001) surfaces correspondingly. Hardness is determined as a relation of the reaction force to the vertical projection of the contact area under conditions of a fully developed plastic zone.

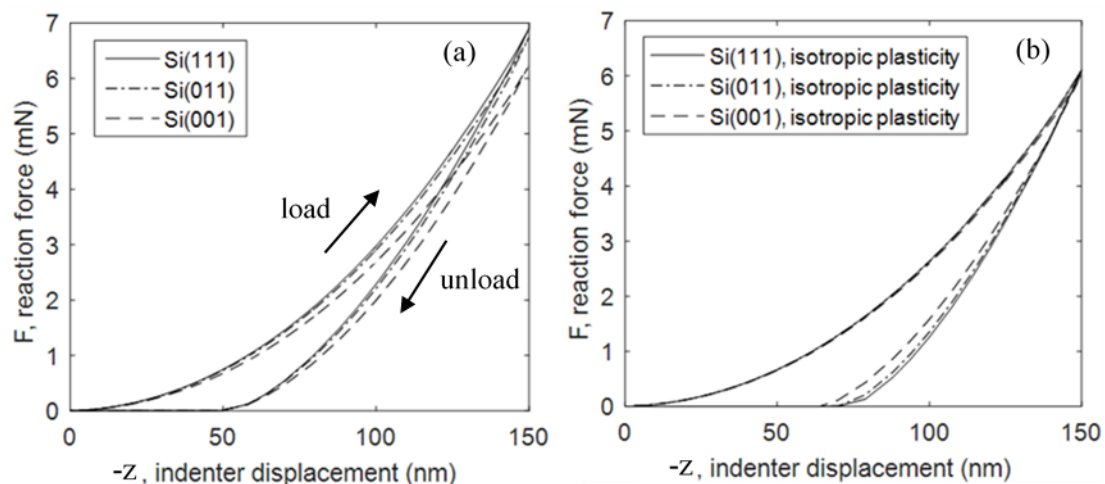


Figure 3. Loading-unloading curves of FEM-computed nanoindentation of different silicon surfaces for (a) anisotropic plasticity and (b) isotropic plasticity, Hill's parameter $h = 1$.

4. Indentation and scratching with spherical tip

A spherical tip, as the most suitable and safe for scratching tests, has been modelled with 25 μm radius of curvature. The spherical indenter exhibits the same hardness differentiation for various surfaces of Ge, Si [5], SiC materials as the Berkovich indenter. It is clear that nonzero component of the reaction force resistant to the direction of the scratching appears (figure 4(a)), but another lateral force may

appear as well. In the case of anisotropic plasticity, even elastically isotropic (111) plane (stiffness tensor is invariant upon any rotation around the cubic [111] axis) loses its symmetry, so that different directions of the scratching produce different plastic strain zones (figure 4(b)). The difference in normal components of the reaction force between the scratch indentation and the usual one is small, but noticeable (figure 5).

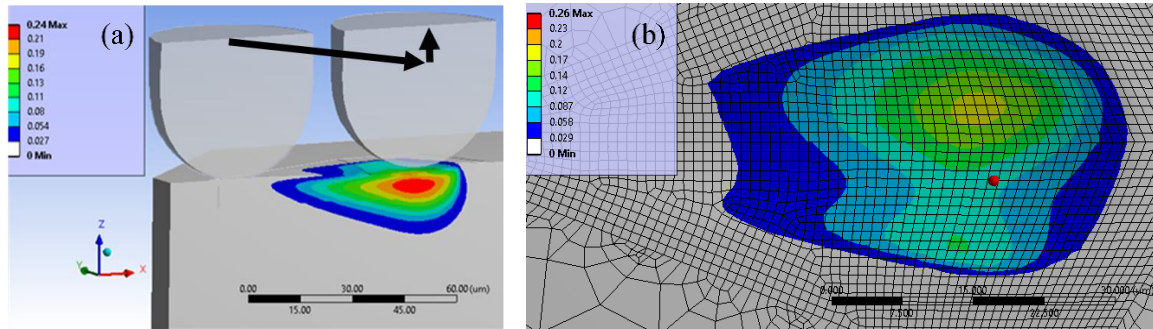


Figure 4. Residual plastic strain (in color) after indentation of Ge(111) surface by 6 μm with concurrent scratching by 60 μm (a) along the $[2\bar{1}\bar{1}]$ axis (section view across symmetry plane) (b) along the axis rotated by 30° from the $[2\bar{1}\bar{1}]$ axis (normal view showing asymmetry in the case of anisotropic plasticity).

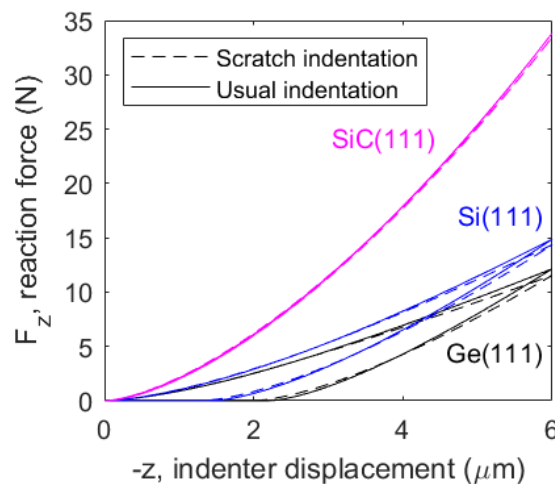


Figure 5. Z-component of the reaction force for indentation with a 25- μm spherical tip compared to the same indentation with concurrent scratching by 60 μm . The loading-unloading curve for SiC is almost fully elastic.

5. Conclusions

Introduction of anisotropic plasticity with the Hill's parameter $h > 1$ into finite-element calculation of indentation of diamond-like crystals Ge, Si, SiC has led to the correct hardness differentiation between the (111), (011) and (001) orientations of the crystals. Various aspects imposed by anisotropic plasticity on indentation and scratching tests have been graphically demonstrated.

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