

Solid-phase homoepitaxy at tribological interfaces between silicon crystals

Thomas Reichenbach^{1,2)*}, Gianpietro Moras¹⁾, Andreas Klemenz¹⁾, Lars Pastewka³⁾, and Michael Moseler^{1,2)}

¹⁾Fraunhofer Institute for Mechanics of Materials IWM, MicroTribology Center μ TC, Freiburg, Germany

²⁾Institute of Physics, University of Freiburg, Germany

³⁾Department of Microsystems Engineering IMTEK, University of Freiburg, Germany

*Corresponding author: thomas.reichenbach@iwm.fraunhofer.de

By means of molecular dynamics simulations of diamond-cubic silicon we show a proof-of-principle of a novel concept to grow crystalline silicon nanostructures with high precision and without the need of elevated temperatures or impurities. The concept exploits shear-induced amorphization and recrystallization processes occurring at sliding contacts between two differently oriented silicon crystals. We explore the origin of this shear-induced homoepitaxial growth and relate it to the anisotropic mechanical properties of silicon crystals.

Keywords: tribology, silicon, molecular dynamics, nanolithography, epitaxy

1. Introduction

Tribologically driven nanolithography of crystalline silicon structures is a novel concept that could shape future electronic applications. The recrystallization of amorphous silicon on a crystalline silicon substrate, so-called solid-phase epitaxial growth, relies so far on temperature often combined with the introduction of doping atoms. As alternative to temperature, shear could provide the atomic mobility necessary for recrystallization. Here, using reactive molecular dynamics simulations, we show a proof-of-principle that this combination of nanotribology and solid-phase epitaxial growth could become a new nanolithography technique that allows for the fabrication of crystalline silicon nanostructures.

2. Results and Discussion

In our previous work, we showed that an amorphous layer forms at sliding interfaces between two silicon crystals [1]. The thickness of such layer reaches a steady state value, where continuously ongoing amorphization and recrystallization processes, both driven by shear, mutually cancel each other out. For identically oriented crystals, the position of the interface layer moves stochastically. However, upon rotation of the two crystals with respect to each other, sliding takes place along different crystallographic directions for the two crystals. In this case, we observe that the amorphous interface still maintains a constant thickness but its position can drift in a specific direction, resulting in the growth of one crystal at the expense of the other crystal (see Fig. 1).

Despite different recrystallization and amorphization kinetics of differently oriented crystals, we find that elasticity alone determines the growth direction in these sliding contacts. More precisely, the crystal with the lower elastic energy density under elastic shear deformation grows. Hence, a reliable prediction of the growth direction is possible by simple-shear deformations of individual crystals or even analytically using linear elasticity.

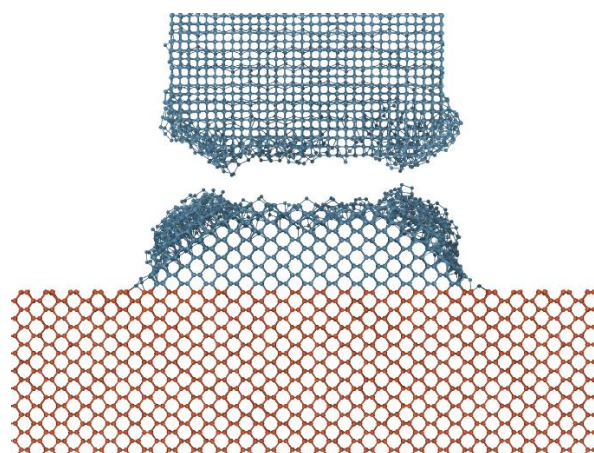


Figure 1: Triboepitaxial growth on an extended Si substrate in contact with a single asperity after sliding and subsequent lifting off the asperity. The color of the atoms refers to the crystal they belonged to prior to sliding (red substrate, blue asperity).

Furthermore, we provide evidence that differences in the shape and size of the crystals in contact can influence the elastic response and thus also the growth direction. We show that this triboepitaxial growth is a general phenomenon occurring for a variety of silicon surface orientations; the only exceptions found are contacts involving (111) surfaces, where the amorphization/crystallization kinetics hinders interface migration. Based on these results we propose an experimental setup to verify our findings and to fabricate arbitrarily shaped crystalline silicon nanostructures on a crystalline silicon substrate.

3. References

- [1] Moras, G. et al., "Shear melting of silicon and diamond and the disappearance of the polyamorphic transition under shear," *Phys. Rev. Materials* 2, 2018, 083601.