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Kinetic Monte Carlo method for the simulation of anisotropic wet etching of quartz

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ABSTRACT

This study combines wet etching experiments and Kinetic Monte Carlo simulations to describe anisotropic etching of quartz for the manufacture of microelectromechanical systems (MEMS). Based on the particular atomistic structure of quartz we introduce a 'quartz-based' removal probability function with nine energy parameters. This enables describing the removal rate of any surface atom as an explicit function of the number of neighbors. An evolutionary algorithm is used to systematically transform the experimental (facet specific) etch rates of nine crystal planes parallel to the X (electric) and Y (mechanical) axes into suitable values for the nine energy parameters. To improve the computational efficiency of the evolutionary search we make use of a transformation matrix, effectively constraining the evolutionary search space. This leads to successful predictions for the etch rates of a wide range of crystallographic facets as well as for the three-dimensional etched shapes obtained on masked Z-cut substrates.

1. Introduction

Like silicon, quartz is widely used in the fabrication of microelectromechanical systems (MEMS). This is due to quartz's outstanding piezoelectric properties, good electric insulation, satisfactory ultraviolet (UV) optical transmission and exceptionally stable, high frequency resonance behavior in a wide temperature range. These features have favored the utilization of quartz as a substrate for the fabrication of several types of MEMS, such as resonators for timing and local-to-global synchronization purposes [1–3], tuning-fork probes for scanning microscopies [3,4] and tuning-fork gyros for angular rate sensors [3,5–7], including other applications as well [8]. Although alternative piezoelectric materials, such as langasite (or LGS), can be utilized for similar purposes [9,10], quartz has the advantage of accuracy [7] in addition to availability [5]. Quartz gyros are specially appreciated for tactical defense applications, including flight attitude control, guidance and positioning, due to their unmatched precision, low power consumption, low cost, exceptional stability over temperature and high resistance to shock [5,6].

The Kinetic Monte Carlo (KMC) method is suitable to study complex fabrication processes leading to the propagation of multivalued surfaces, playing an important role in the simulation of the microstructure and morphology during anisotropic etching of silicon for the fabrication of MEMS [11–15]. In spite of this, the KMC method has never been applied to describe the anisotropic etching of quartz. This is due to the more complex atomistic structure of quartz. In fact, while research in both the underlying etching mechanism [16–25] and complementary modeling methods [15,26–32] are well developed for silicon, the equivalent for quartz is lagging behind, in spite of significant efforts on both the experimental and computational approaches [33–41].

Belonging to the trigonal system, quartz is characterized by a high stability against chemical reactions with other substances. In the case of the micromachining of quartz-based MEMS, wet etching in saturated NH_4HF_2 is one of the most widely used methods, benefitting from similar features as silicon etching: low cost, the emergence of flat surfaces, sensitivity to temperature and solu-

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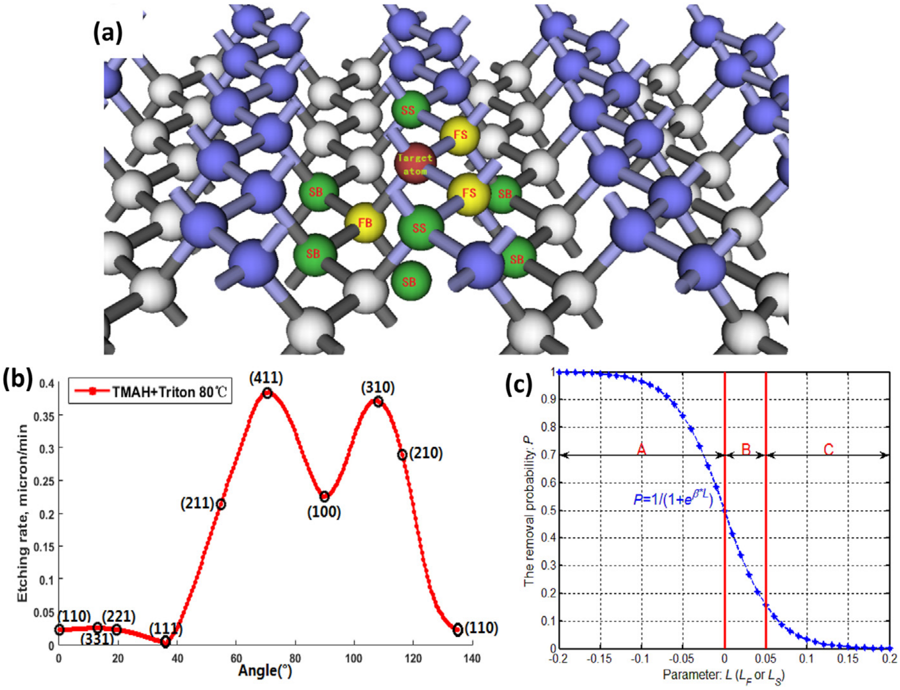

Fig. 1. (a) Atomistic structure of the ideal crystallographic cut of Si(110); (b) Typical etch rates for crystalline silicon in 25 wt% TMAH + 0.1 vol% Triton at 80 C. The plot shows the rates for the main silicon orientations—(100), (110) and (111) —as well as for various vicinal planes located between them. (c) Removal probability *p* as a function of the excess energy *L*, displaying the three regions A, B and C for high, medium and low probability, respectively, as considered in the Si-RPF model (see main text). (a)–(c) after Ref. [15].

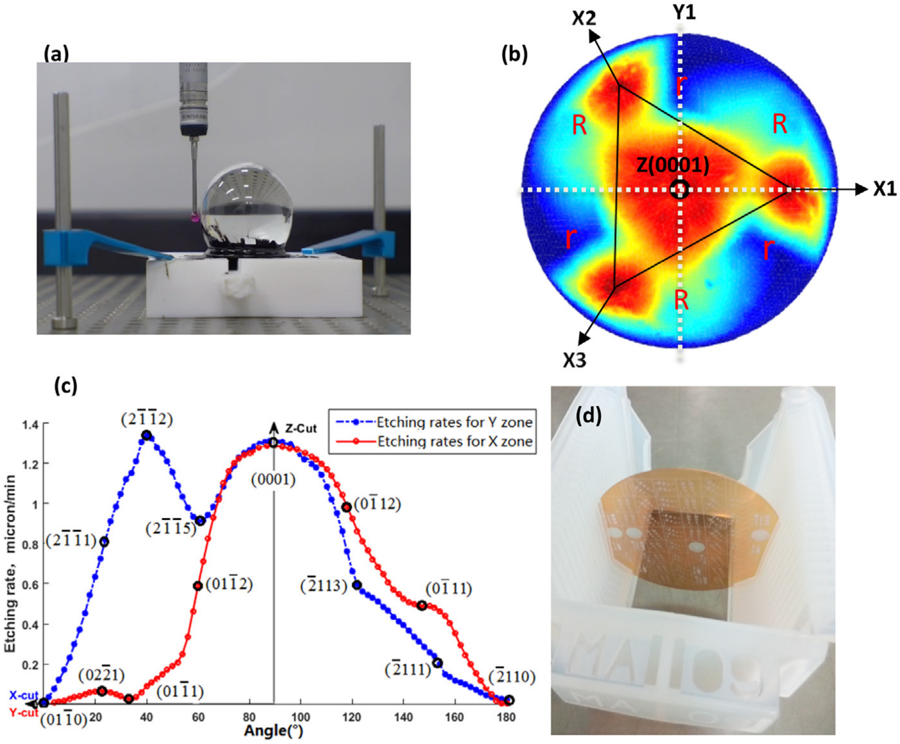

Fig. 2. (a) Optical image of a typical, polished quartz hemisphere used in our wet etching characterization experiment; (b) Etch rate distribution in saturated NH_4HF_2 solution at 80C for a hemisphere etched for 95 min. (c) Corresponding etch rates for the X and Y crystallographic zones. [For a given direction [hkml], the crystallographic zone of [hkml] contains all the crystallographic planes parallel to that direction.]. (d) Z-cut quartz wafer with Cr/Au mask.

tion concentration, and the possibility of batch processing [36,37]. Although the complex anisotropy of the etching process has been characterized in multiple studies, only limited efforts have been made in order to obtain reliable models that properly describe the etching anisotropy, 3D structure and surface morphology of quartz [33,36–39]. The existing Level Set (LS) method shows a tendency to generate rounder features at the intersection of planes in convex corners and mesa structures (see e.g. Fig. 5(c) and (f) in