X-ray scattering study of the Ge(001):Te 1 x 1 surface structure

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Introduction

Tellurium has proven to be an effective surfactant in forming a sharp interface in Ge/Si heteroepitaxial structures grown by molecular beam epitaxy (MBE) [1]. To understand this growth mechanism on an atomic scale, structural parameters such as adsorption sites and bond lengths for both Te on Si(001) and Te on Ge(001) are important prerequisites. Using x-ray standing waves (XSW) and low-energy electron diffraction (LEED), Lyman and associates [2] made an atomic scale study of the Te/Ge(001) surface. For the 1 ML Te/Ge(001) surface, the (004) and (022) XSW coherent positions triangulated the Te positions relative to the Ge bulk lattice and found them to be consistent with a two-fold bridge. The observed reduction in the XSW (022) coherent fraction was shown to agree with the expected Te lateral displacements from the bridge sites in the missing-row model (Figure 1) due to the misfit between the Ge and Te overlayer. Our goal in this first ultrahigh vacuum (UHV) surface study at the Advanced Photon Source (APS) was to determine surface relaxations for the Te atomic layer and the top Ge atomic layers of the Ge(001):Te 1 x 1 surface structure using x-ray crystal truncation rod (CTR) measurements [3]. Comparatively speaking, x-ray scattering measurements are more sensitive to disorders such as relaxation and vacancies, while XSW measurements give the exact adsorbate position with respect to the bulk atomic planes.

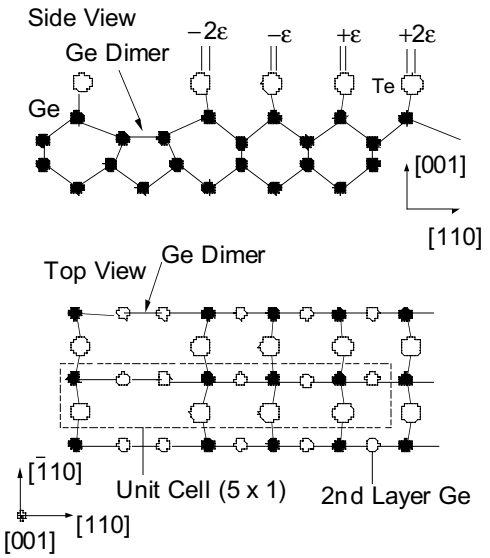

Figure 1: Te missing-row model for the Ge(001):Te 1 x 1 surface.

Methods and Materials

The experiments were carried out in a UHV surface chamber that is part of an x-ray diffractometer [4] at the 5-ID-C station on the DuPont-Northwestern-Dow (DND-CAT) undulator beamline. The UHV chamber has surface preparation capabilities including ion sputtering, annealing, and solid source MBE, as well as surface analysis via LEED, Auger electron spectroscopy , XSW, surface extended x-ray absorption fine structure, and surface x-ray scattering. Its base pressure was 2.5 x 10^{-10} torr. The sample was prepared by a similar method as previously reported for Ge(001):Te 1 x 1 [2]. This included Te deposition at a substrate temperature of 270°C followed by annealing to 415 °C. After Te deposition, we observed a 1 x 1 LEED pattern with streaks between the 00 and 01 spots. This indicates that the surface had 1 x 1 long-range order but was locally disordered.

The 18.0 keV incident x-ray beam was prepared by using the third harmonic of the undulator and the liquid-nitrogen-cooled double-crystal Si(111) beamline monochromator. A pair of beamline horizontally deflecting mirrors were set to reject harmonics and to horizontally focus the monochromatic beam. We recorded scattered intensities along the 1 0 L , 11 L , and 3 0 L crystal truncation rods with the incident angle fixed at 0.5°. (The critical angle for total external reflection of 18 keV x-rays reflecting from Ge is 0.14°.) The net counts at each point along a CTR were obtained from a transverse scan through the CTR with linear background subtraction [5]. One of the weakest intensities at L = 1.75 in the 1 0 L scan was 2.1 x 10^4 counts/s/mm^2. The Lorentz, polarization, and geometrical corrections were then made [5].

Results and Discussion

Based on the in-plane XSW measurement [2], we introduce symmetric displacements of Te lateral positions (expressed as ε and 2ε in Figure 1). The XSW value of ε is 0.058 • *a* where *a* is surface unit cell length (4.001 Å). We fit the Te missing-row model (Figure 1) to the CTR data to refine the vertical displacements of the Te atom layer and the first four Ge atomic layers. We also used the Rutherford backscattering spectroscopy (RBS) to measure Te coverage (0.74 ML) [6]. The isotropic vibrational amplitudes used in the fit were $(\langle u^2\rangle_{Te})^{1/2}$ = 0.13 Å and $(\langle u^2\rangle_{Ge})^{1/2}$ = 0.10 Å. After allowing vertical relaxation (and using the value of the lateral displacements predicted from the XSW measurements), the CTR χ^2 is 1.39. The fitted curves are shown in Figure 2 as solid lines. In this model, the displacement of the Te atomic layer along the *Z* direction from the bulk Ge position is + 0.115 Å, where + sign

stands for atoms shifted outward. The first through fourth Ge atomic layers are shifted vertically by -0.021, -0.029, +0.004, and -0.002 Å, respectively, from the bulk Ge positions. The Te-Ge bond length is 2.57 Å and 2.54 Å, for the 2ε displacement Te and ε displacement Te, which is comparable to the sum (2.54 Å) of Pauling tetrahedral atomic radii [7]. The Te position agrees to within 0.016 Å with the XSW result [2]. The obtained surface roughness is 2.12 Å.

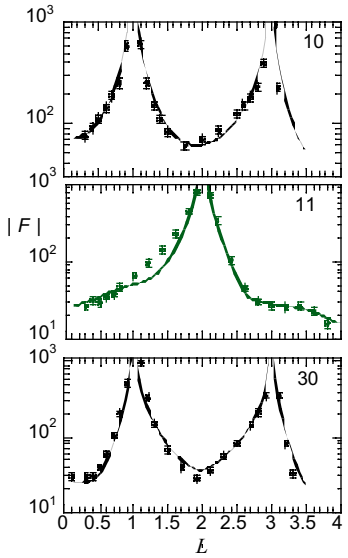

Figure 2: Structure factors measured along the 1 0 L, 11 L, and 3 0 L CTEs for the Ge(001):Te 1x 1 surface. The hkl indices are based on a tetragonal unit cell with a base defined by the 1 x 1 surface unit cell of Ge(001).

Acknowledgments

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