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INTRA-CASCADE SURFACE RECOMBINATION OF POINT DEFECTS
DURING ION BOMBARDMENT OF Ge (001)

J. A. Floro, B. K. Kellerman, E. Chason, S. T. Picraux, D. K. Brice, and K. M. Horn, Sandia National Laboratories, Albuquerque, NM 87185.

ABSTRACT

Low energy Ar and Xe ion bombardment of Ge (001) produces large numbers of point defects on the Ge surface and in the near-surface regions. Defect concentrations on the surface are detected and quantified in real time during bombardment using *in situ* Reflection High Energy Electron Diffraction (RHEED). We report the energy dependence of the defect yield for 70-500 eV Ar and Xe ion bombardment, and the temperature dependence of the defect yield (defects/ion) during 200 eV ion bombardment. The defect yield drops rapidly as the substrate temperature during bombardment is varied from 175 K to 400 K. We attribute the yield reduction to surface recombination of adatoms and vacancies produced in the same collision cascade.

INTRODUCTION

Ion bombardment during film deposition can significantly modify the morphology of epitaxial growth surfaces through creation of non-equilibrium surface (and bulk) point defect populations.[1-3] In this context, beam generated point defects can modify the growth surface morphology during epitaxial growth. On the other hand, minimizing residual damage due to bombardment is a concern both in film growth and in plasma processing steps used in microelectronic device fabrication. In this study we quantify surface defect production and examine the temperature dependence of the observed defect production yield. Increasing temperature greatly reduces the observed yield. A simple model based on intra-cascade surface recombination is discussed.

EXPERIMENT

A detailed description of the experimental technique may be found in ref. [4] -- only a brief description is given here. The experimental arrangement is shown inset in Fig. 1. All measurements were performed in a turbo-pumped UHV chamber with a 1×10^{-10} Torr base pressure. Smooth surfaces on undoped Ge (001) single crystals were prepared by repeated cycles of sputter cleaning with 500 eV Xe at temperatures less than -25°C , followed by 725°C , 5 minute annealing. The clean surface evinces a primary 2×1 reconstruction measured by RHEED, with secondary $p\text{-}2 \times 2$ and $c\text{-}4 \times 2$ reconstructions [5].

The sample was bombarded with Ar or Xe ions in the 70-500 eV energy range from a sputter ion gun at 60° off-normal angle of incidence. The maximum ion current density was 50 ± 10 nA/cm². Accurate measurement of the ion current is critical to obtaining correct values for the defect yield. In these experiments the ion current is measured directly on the Ge substrate, which is exposed to the ion beam through a grounded shield with a collection area-defining aperture. The ground shield is below the plane of the substrate surface to prevent sputter contamination of the Ge. Secondary electron emission, fast neutrals, and doubly charged ions were all found to be negligible [4].

Surface roughening is measured by monitoring the intensity of the out-of-phase specular RHEED spot. In this condition, destructive interference occurs between atoms on adjacent levels of the surface, yielding high sensitivity to sub-monolayer roughness. For details, see refs. [6,7]. For randomly distributed roughness, the specular RHEED intensity is given by [7]:

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Figure 1. RHEED intensity during Ar bombardment of Ge at 200 eV and 500 eV. Solid lines are fits of equation 1 to the data. The experimental setup is depicted schematically, inset.

$$\frac{I}{I_0} = e^{-\theta}, \theta = \frac{Y_D J t}{n_s} \quad (1)$$

where θ is the defect coverage expressed in monolayers, Y_D is the defect yield (ion^{-1}), J is the ion current density, t is time, and n_s is the monolayer atomic density of Ge (001), $n_s = 6.25 \times 10^{14}$ atoms per cm^2 . The defect coverage θ is obtained by fitting equation 1 to the intensity vs. time curves. An example is shown in Fig. 1. The intensity has had the background due to inelastic scattering subtracted out. Finally, we emphasize that this technique for measuring defect production is *purely surface sensitive*, i.e., the RHEED beam only detects defects that reside on the surface of the sample and ignores those in the bulk.

RESULTS

Figure 2 shows the dependence of the Ge surface defect yield on ion energy for Ar and Xe bombardment. The substrate temperature was maintained at about -100°C . Copious defect production yields are observed, with $Y_D \approx 30$ defects/ion for 500 eV Ge bombardment. In order to further interpret the data, the cascade process was simulated using binary collision calculations in our modified version of the TRIM simulation code that we refer to as TRIMRC [8]. A bulk displacement threshold energy of $E_D^b = 15$ eV was used for the calculations [9] and a surface displacement threshold energy of $E_D^s = 11.25$ ($0.75 E_D^b$) was assumed. For purposes of comparison with the data, we partition the simulation results into three categories, as depicted schematically in Fig. 3: (1) total defects - the sum of all vacancies and interstitials (which will be called adatoms if they are on the surface), both on the surface and in the bulk, produced per ion; (2) surface defects - all defects that reside in the first three monolayers after the cascade has quenched; (3) sputtering - all events in which an atom goes to infinity leaving only a surface vacancy. Note that the number of vacancies equals the number of interstitials plus the number of sputter events. For Xe and Ar it is found that the experimental yield exceeds the predicted *total* defect yield over the entire 70-500 eV energy range.

Figure 4 shows the temperature dependence of the observed Ge (001) surface defect creation yield for 200 eV Ar and Xe ion bombardment. At low temperatures the yield during Ar and Xe bombardment is about equal to the total defect yield (as discussed above), whereas at elevated temperatures the yield is much lower and is about equal to the sputter yield (≤ 1 defect/ion [10]). The change in the observed yield occurs over a 150 K region roughly centered on room temperature.

Figure 2. Experimental defect yields vs ion energy for 200 eV (a) Ar and (b) Xe ions on Ge (001) at -100°C . Also shown are the predictions of TRIMRC for total defects (TD), surface defects (SD), and sputtering (SP).

Figure 3. Schematic cross-sectional view of Ge sample showing cascade defects.

DISCUSSION

The data of Fig. 2 shows that the surface point defect yield detected by RHEED exceeds the total predicted defect yield over the 70-500 eV energy range. At 500 eV, TRIMRC indicates that the post-cascade point defects are distributed within the first

16 monolayers below the surface. Detection of these defects by RHEED thus implies that defects created in the bulk are migrating at -100°C . Mobility of the point defects at -100°C is consistent with previous reports of low activation energies for migration of vacancies and interstitials in Ge and Si ($Q_{\text{mig}} \approx 0.15 - 0.4 \text{ eV}$ [11]). Alternatively, TRIMRC may simply overestimate the cascade depth. Further discussion may be found in ref. [4].

We believe the decrease in the observed surface defect yield with increasing temperature (Fig. 4) results from defect annealing *on the Ge surface*, rather than in the bulk. While increasing the temperature increases the bulk diffusivity, this will enhance the rate at which defects reach the surface, as well as the bulk recombination rate of vacancies and interstitials. Thus the fraction of the defects generated per cascade that reach the surface should be relatively insensitive to temperature. Once on the surface, however, the defects can diffuse and either recombine with each other, or can annihilate at ledge sites. Activation energies

Figure 4. Temperature dependence of the observed defect yield. The inverted triangles are from the data of Chason *et al* [12]. The solid line is a fit of equation (2).

for surface diffusion of 0.8 eV were measured during 200 eV Xe bombardment of Ge by Chason *et al* [12]. In the temperature range used here, the defects do not have sufficient surface mobility to reach ledge sites and are only capable of short range surface diffusion. One picture of the behavior of point defects after the cascade, depicted schematically in Fig. 5, is as follows: the defects created by a given collision cascade diffuse to the surface to become adatoms and surface vacancies. Inasmuch as the cascade is relatively shallow, the surface defects will lie relatively close to one another. An estimate of the initial defect separation is $R_i = (A_{cas}/Y_D)^{1/2}$. Taking the cascade radius to be 11 monolayers (equal to the maximum cascade depth determined by TRIMRC), we obtain $R_i = 8.5 \text{ \AA}$. At very low temperatures ($\leq 200 \text{ K}$) the surface defects are immobile due to the large activation energy for surface diffusion, and surface recombination is suppressed. The number of surface defects is therefore equal to the total number of created defects. At somewhat higher temperatures, the defects gain sufficient mobility to diffuse the short distances necessary for recombination with opposite type defects created in the same cascade, resulting in an apparent reduction in the measured defect yield. At temperatures approaching 400 K, this process goes to completion, i.e., all adatoms recombine with surface vacancies, leaving behind only the uncompensated vacancies created by sputtering events. Finally, further increasing the temperature results in the remaining vacancies gaining sufficient mobility to diffuse to ledge sites and annihilate.

Ledge annihilation was observed by Chason *et al*, who measured the temperature dependence of the defect yield during 200 eV Xe ion bombardment of Ge (001) at temperatures from 500-700 K. In this range they found that the surface reaches a temperature-dependent steady-state roughness. They modeled the steady-state behavior on the basis of competition between defect production and defect annealing via surface diffusion to ledges. Fits of this model to the data predict an activation energy for surface diffusion of 0.8 eV, as mentioned above. Furthermore, they determine a defect production yield of about 1 defect per Xe ion, consistent with our results, showing that at these temperatures only the sputter vacancies survive recombination. The data of Chason *et al* is also shown in Figure 4.

The temperature dependence of the surface defect yield as shown in Figure 4 may be simply modeled by writing the observed yield as

$$Y_{\text{obs}} = Y_{\text{sput}} + \frac{(Y_t - Y_{\text{sput}})^2}{Y_t - Y_{\text{sput}} + \frac{n_s D}{J_i R^2}}, \quad (2)$$

where Y_{sput} is the sputter yield, Y_t is the total defect yield, D is the surface diffusivity, $D = D_0 \exp(-Q_{\text{surf}}/kT)$, and R is the average interdefect separation on the surface. D/R^2 thus represents the annealing rate (#/s) and the prefactor n_s/J converts this rate to a yield. Inasmuch as the data are sparse, and since TRIMRC predicts Ar and Xe have similar total defect and sputter yields, we treat the Ar and Xe data points of Fig. 4 as a single data set for purposes of fitting equation 2. The fit is performed by enforcing $Q_{\text{surf}} = 0.8$ eV from Chason *et al*, and $Y_{\text{tot}} = 10.5$ from the data, and allowing Y_{sput} and $n_s D_0/JR^2$ to vary in a non-linear least squares algorithm. The resulting best fit is shown as the solid line in Fig. 4. The values of the fitting parameters are $Y_{\text{sput}} = 1.04$ defects/ion and $n_s D_0/JR^2 = 7 \times 10^{14}$. Taking $n_s = 6.24 \times 10^{14}$, $J = 50$ nA/cm², and $D_0 = 10^{-3}$ s⁻¹, we get an average interdefect separation of 5.5 Å. Despite the crudeness of the model, reasonable behavior is obtained. Clearly, however, the data shown in Fig. 4 are insufficient to impute high confidence in the details of the model. In particular, much lower substrate temperature needs to be obtained to verify that the observed defect yield saturates at the total defect yield as predicted.

The model presented above for the temperature dependence of the defect yield has implications for beam assisted epitaxial growth. At typical growth temperatures a yield of only about one defect per ion is measured for Ar and Xe bombardment of Ge. However, the data and model suggest that more than an order of magnitude more defects are present *transiently* on the surface prior to recombining with one another. These defects, if present during the dynamic growth process, can modify the cluster size distribution, affecting film smoothness and morphology [2,3,13].

Figure 5. Plan view of the Ge (001) surface showing the temperature-dependent stages of surface annealing of point defects all created in the same collision cascade.

Summary

70-500 eV Ar and Xe ion bombardment of the Ge (001)-2x1 surface produces adatoms and surface vacancies that are detected *in situ* in real time by monitoring the intensity of the out-of-

phase specular RHEED spot. At substrate temperatures of -100°C the measured surface defect yields are as high as 30 defects per ion for 500 eV Xe bombardment. Over the entire 70-500 eV range of ion energy the measured yield for both Ar and Xe exceeds the total defect yield (surface plus bulk) predicted by TRIMRC. At elevated substrate temperatures the observed surface defect yield is reduced, presumably by defect annealing. Because the surface diffusivity is too low for defect annihilation at ledge sites, we argue that the annealing arises from direct surface recombination of point defects that lie within a few lattice constants of one another, and thus must all arise from the same cascade. At sufficiently high temperatures only the number of defects corresponding to the sputter yield is measured. However, much larger point defect densities may transiently reside on the surface which, in the context of beam enhanced epitaxial growth, can modify the growth surface and cluster morphology.

Acknowledgments

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